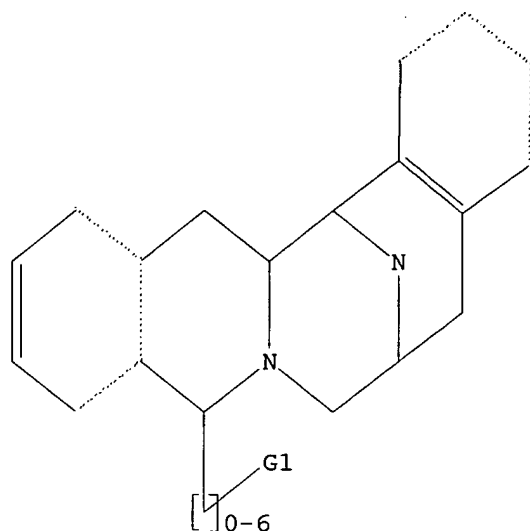


10/826,859

R



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l4

SAMPLE SEARCH INITIATED 19:07:38 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 38 TO ITERATE

100.0% PROCESSED 38 ITERATIONS  
SEARCH TIME: 00.00.01

4 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 391 TO 1129  
PROJECTED ANSWERS: 4 TO 200

L5 4 SEA SSS SAM L4

=> s l4 sss full

FULL SEARCH INITIATED 19:07:47 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 695 TO ITERATE

100.0% PROCESSED 695 ITERATIONS  
SEARCH TIME: 00.00.01

92 ANSWERS

L6 92 SEA SSS FUL L4

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE  
ENTRY

TOTAL  
SESSION

FULL ESTIMATED COST

323.09

323.30

FILE 'CAPLUS' ENTERED AT 19:07:54 ON 15 FEB 2005  
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10/826,859

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FILE COVERS 1907 - 15 Feb 2005 VOL 142 ISS 8  
FILE LAST UPDATED: 14 Feb 2005 (20050214/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l6

L7 26 L6

=> d l7 1-26 ibib abs hitstr

L7 ANSWER 1 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:680266 CAPLUS

DOCUMENT NUMBER: 141:167764

TITLE: Renieramycins, their isolation from Xestospongia species, and anticancer agents containing them

INVENTOR(S): Kubo, Yotoku; Saito, Naoki; Pummangura, Sunibhond; Suwanborirux, Khanit

PATENT ASSIGNEE(S): Chulalongkorn University, Japan; National Center for Genetic Engineering and Biotechnology; National Science and Technology Development Agency

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

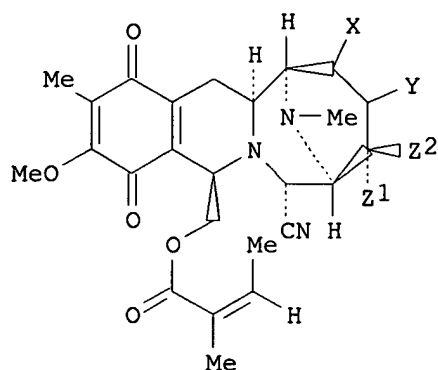
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004231552	A2	20040819	JP 2003-20821	20030129
PRIORITY APPLN. INFO.:			JP 2003-20821	20030129
OTHER SOURCE(S):	MARPAT	141:167764		
GI				



I

AB Renieramycins I [XY = COC(OMe):CMeCO, C(OH):C(OMe)CMe:C(OH); Z1, Z2 = H, OH, C1-6 alkoxy, acetoxy; Z1Z2 = O] are isolated from blue sponge of Xestospongia sp. via homogenization, treatment with KCN while adjusting pH to 5.5-7.5 using phosphate buffers, extraction with MeOH, and purification by chromatog. Renieramycin M [I; XY = COC(OMe):CMeCO, Z1 = Z2 = H] in vitro inhibited human pulmonary cancer cells QG 56 with IC50 of 1.9, vs. 5.5, for saframycin A.

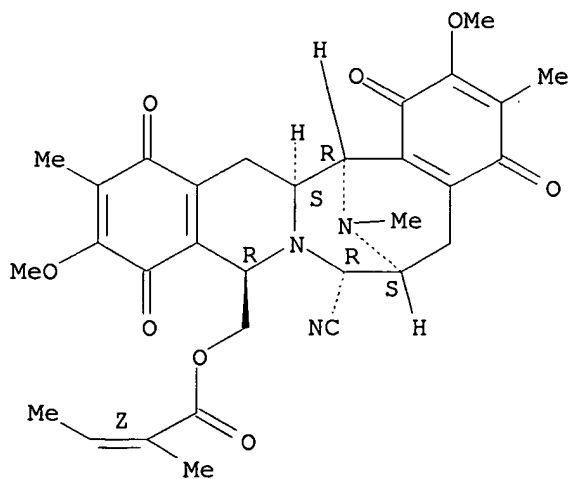
IT 631913-64-9P, Renieramycin M 631913-65-0P, Renieramycin N

RL: PAC (Pharmacological activity); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(anticancer agents containing renieramycins from Xestospongia sp.)

RN 631913-64-9 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



RN 631913-65-0 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,7R,9R,14aS,15R)-7-cyano-6,7,9,10,13,14,14a,15-octahydro-1,4,5-trihydroxy-2,11-dimethoxy-3,12,16-

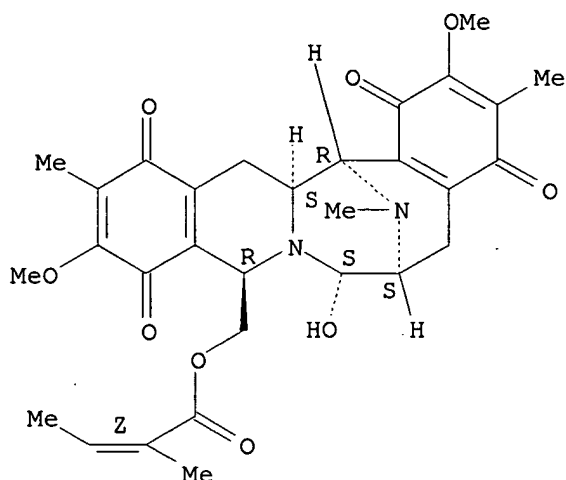
(anticancer agents containing renieramycins from *Xestospongia* sp.)

RN 123641-95-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L7 ANSWER 2 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:595237 CAPLUS

DOCUMENT NUMBER: 142:32489

TITLE: identification of renieramycin A as an antileishmanial substance in a marine sponge *Neopetrosia* sp

AUTHOR(S): Nakao, Yoichi; Shiroyiwa, Takeru; Murayama, Shuhei;  
Matsunaga, Shigeki; Goto, Yasuyuki; Matsumoto,  
Yoshitsugu; Fusetani, Nobuhiro

CORPORATE SOURCE: Lab. Aquatic Natural Products Chem., Grad. Sch.  
Agricultural and Life Sci., The Univ. Tokyo, Tokyo,  
113-8657, Japan

SOURCE: Marine Drugs (2004), 2(2), 55-62

CODEN: MDARE6; ISSN: 1660-3397

URL: <http://www.mdpi.net/marinedrugs/papers/papers04/md202055.pdf>

PUBLISHER: MDPI Center

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB The newly developed assay system using recombinant *Leishmania amazonensis* expressing enhanced green fluorescent protein (La/egfr) has been applied to the screening of Japanese marine sponges for antileishmanial activity. Bioassay-guided fractionation of an active sponge *Neopetrosia* sp. afforded an active compound which was identified as renieramycin A by spectroscopic anal. It inhibited La/egf with an IC<sub>50</sub> value of 0.2 µg/mL.

IT 79664-60-1P, Renieramycin A

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

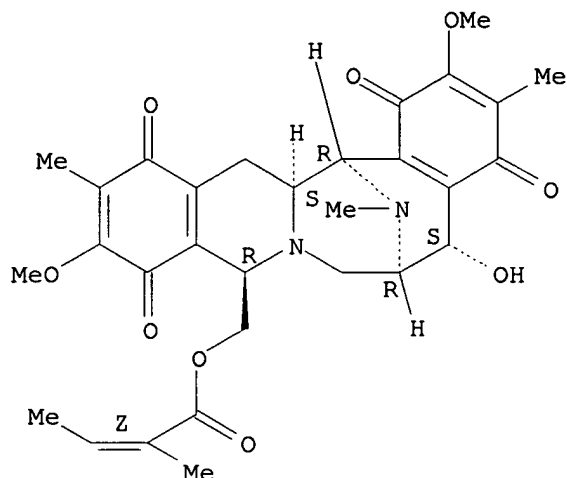
(r)enieramycin A showed dose-dependent inhibition against *Leishmania amazonensis* expressing enhanced green fluorescent protein in new assay.

indicating antileishmanial activity and also showed cytotoxicity  
against P388 murine leukemia cell)

RN 79664-60-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:465167 CAPLUS

DOCUMENT NUMBER: 141:120456

TITLE: Chemistry of renieramycins. Part 5. Structure  
elucidation of renieramycin-type derivatives O, Q, R,  
and S from Thai marine sponge Xestospongia species  
pretreated with potassium cyanide

AUTHOR(S): Amnuoypol, Surattana; Suwanborirux, Khanit;  
Pummangura, Sunibhond; Kubo, Akinori; Tanaka, Chieko;  
Saito, Naoki

CORPORATE SOURCE: Bioactive Marine Natural Products Chemistry Research  
Unit (BMNCU), Department of Pharmacognosy, Faculty of  
Pharmaceutical Sciences, Chulalongkorn University,  
Bangkok, 10330, Thailand

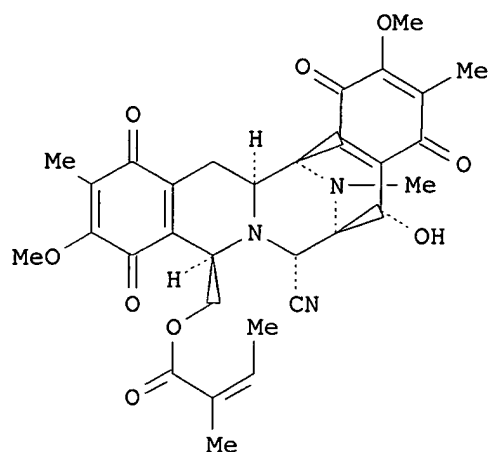
SOURCE: Journal of Natural Products (2004), 67(6), 1023-1028  
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Four minor renieramycin-type derivs., including renieramycins O (I) and Q-S, were isolated from the sponge *Xestospongia* sp. pretreated with potassium cyanide. Their structures were elucidated by comparison of spectral data with those of recently reported renieramycins M and N. The results of transformation and cytotoxicity measurements are also described.

IT **723308-87-0P**

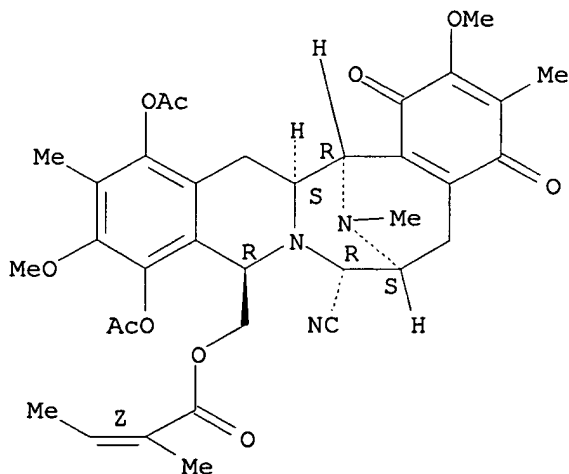
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(antitumor activity of)

RN 723308-87-0 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7R,9R,14aS,15R)-10,13-bis(acetyloxy)-7-cyano-1,5,6,7,9,14,14a,15-octahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4-dioxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



IT **631913-65-0, Renieramycin N**

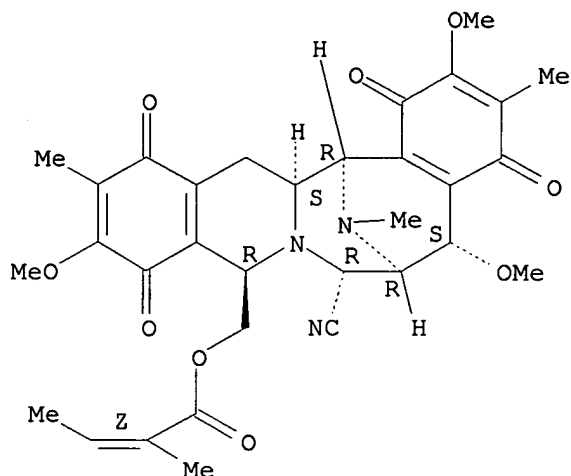
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);

10/826,859

RN 724707-54-4 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-2,5,11-trimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).  
Double bond geometry as shown.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:278842 CAPLUS

DOCUMENT NUMBER: 141:38759

TITLE: Chemistry of renieramycins. Part 6: Transformation of renieramycin M into jorumycin and renieramycin J including oxidative degradation products, mimosamycin, renierone, and renierol acetate

AUTHOR(S): Saito, Naoki; Tanaka, Chieko; Koizumi, Yu-ichi; Suwanborirux, Khanit; Amnuoypol, Surattana; Pummangura, Sunibhond; Kubo, Akinori

CORPORATE SOURCE: Meiji Pharmaceutical University, Kiyose, Tokyo, 204-8588, Japan

SOURCE: Tetrahedron (2004), 60(17), 3873-3881  
CODEN: TETRAB; ISSN: 0040-4020

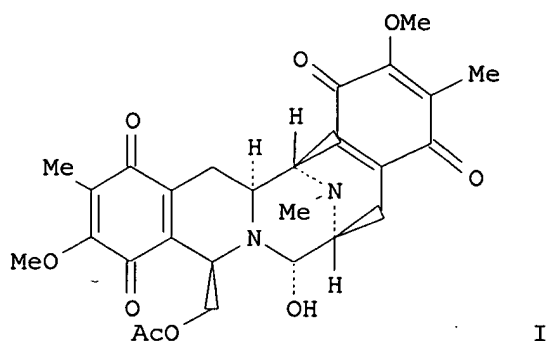
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:38759

GI



AB The transformation of renieramycin M into renieramycin J and jorumycin (I) is presented along with the results of antiproliferative assay data. The chemical stability and the oxidative degradation of I and renieramycin E to generate simple isoquinoline alkaloids, such as mimosamycin, renierol acetate, and renierone are also described. The cytotoxicity IC<sub>50</sub> of jorumycin and derivs. was determined

IT 123641-95-2, Renieramycin e 631913-64-9, Renieramycin M

RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)

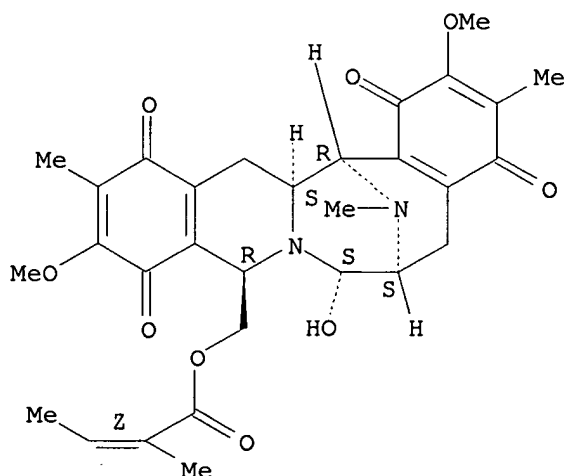
(transformation of renieramycin M into jorumycin and renieramycin J including oxidative degradation products, mimosamycin, renierone, and renierol acetate)

RN 123641-95-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

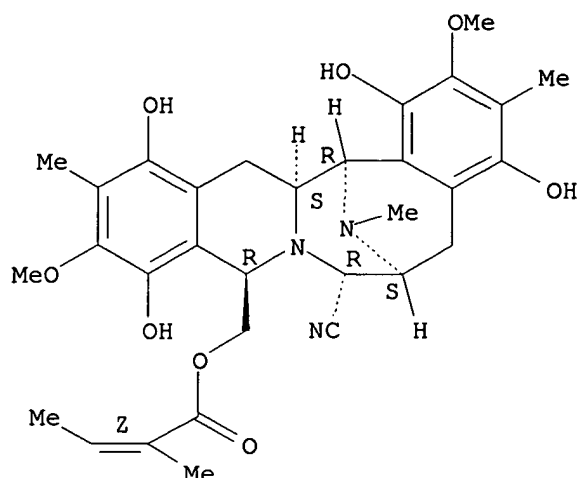
Double bond geometry as shown.



RN 631913-64-9 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)





REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:133034 CAPLUS

DOCUMENT NUMBER: 141:292493

TITLE: Renieramycin P, a highly cytotoxic tetrahydroisoquinoline alkaloid, from a marine sponge *Neopetrosia* sp. [Erratum to document cited in CA139:227487]

AUTHOR(S): Oku, Naoya; Matsunaga, Shigeki; van Soest, Rob W. M.; Fusetani, Nobuhiro

CORPORATE SOURCE: Laboratory of Aquatic Natural Products Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Bunkyo, Tokyo, 113-8657, Japan

SOURCE: Journal of Natural Products (2004), 67(3), 526

CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The term "renieramycin J" should read as "renieramycin P" throughout the paper.

IT **593280-18-3P**

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

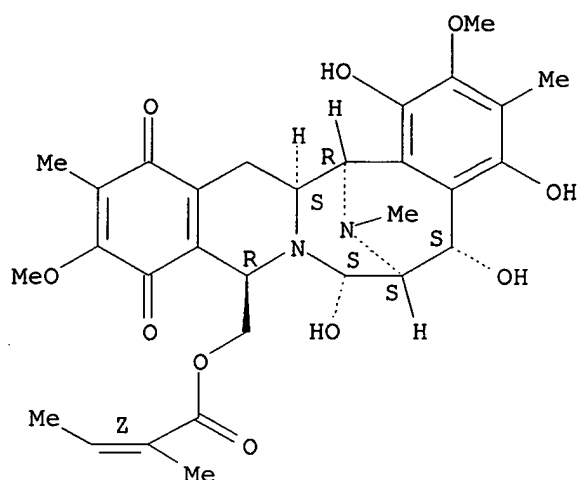
(cytotoxic tetrahydroisoquinoline alkaloid from marine sponge *Neopetrosia* sp. (Erratum))

RN 593280-18-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-6,7,9,10,13,14,14a,15-octahydro-1,4,5,7-tetrahydroxy-2,11-dimethoxy-3,12,16-trimethyl-10,13-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Double bond geometry as shown.



IT 592532-76-8P 592532-77-9P 592532-78-0P

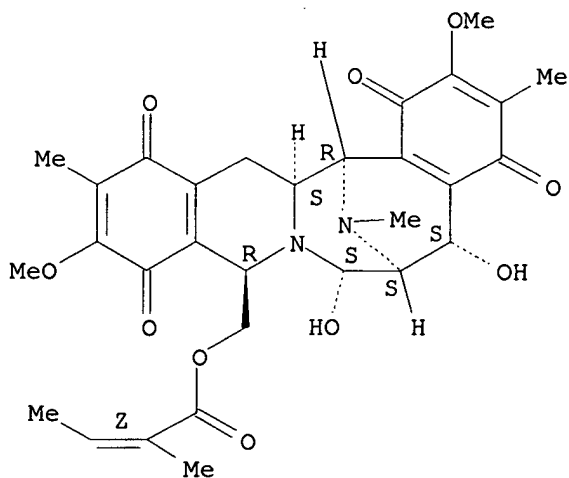
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and properties of (Erratum))

RN 592532-76-8 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5,7-dihydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

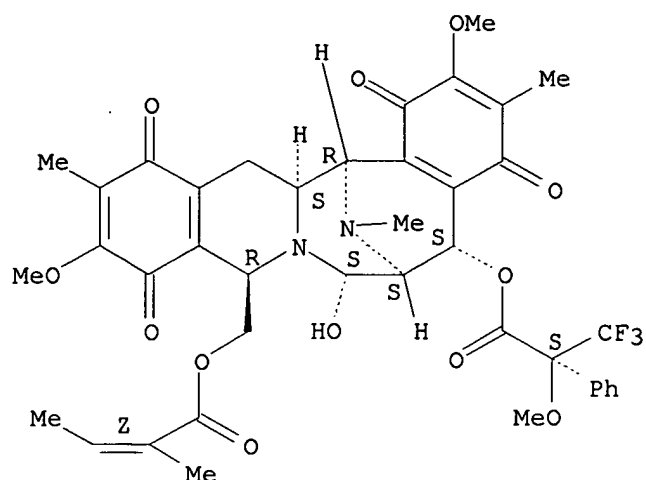


RN 592532-77-9 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-, (5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-9-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-5-yl ester, ( $\alpha$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

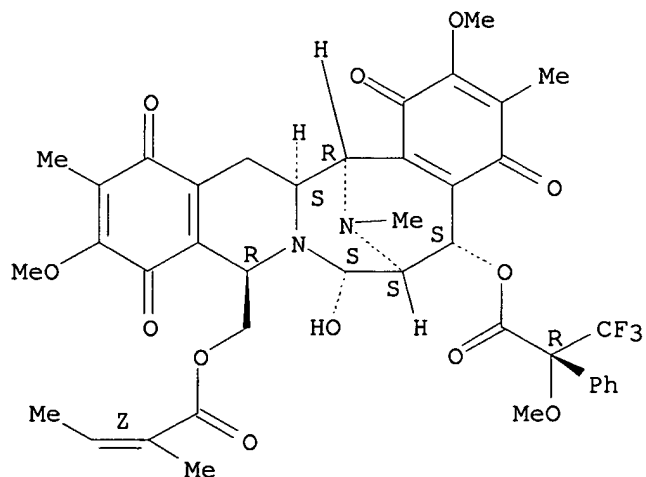


RN 592532-78-0 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -methoxy- $\alpha$ -(trifluoromethyl)-, (5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-9-[[[(2Z)-2-methyl-1-oxo-2-butenyl]oxy]methyl]-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-5-yl ester, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L7 ANSWER 6 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:832855 CAPLUS

DOCUMENT NUMBER: 140:14944

TITLE: Chemistry of renieramycins. Part 3. Isolation and structure of stabilized renieramycin type derivatives possessing antitumor activity from Thai sponge Xestospongia species, pretreated with potassium cyanide

AUTHOR(S): Suwanborirux, Khanit; Amnuoypol, Surattana; Plubrukarn, Anuchit; Pummangura, Sunibhond; Kubo, Akinori; Tanaka, Chieko; Saito, Naoki

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Chulalongkorn University, Bangkok, 10330, Thailand  
 SOURCE: Journal of Natural Products (2003), 66(11), 1441-1446  
 CODEN: JNPRDF; ISSN: 0163-3864  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

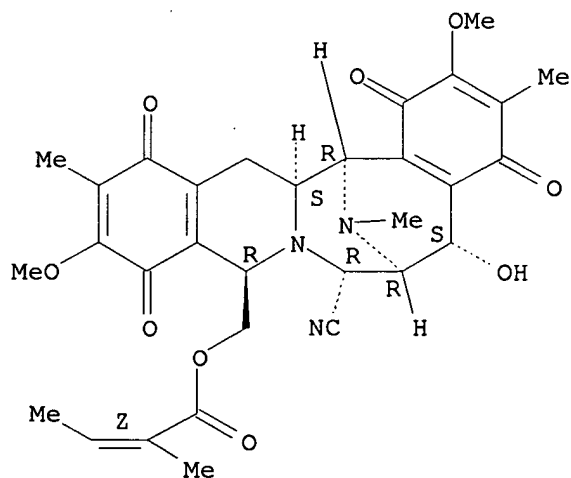
AB Renieramycins M (I) and N (II) were isolated from the Thai sponge *Xestospongia* sp., pretreated with potassium cyanide in methanolic buffer solution, and their structures and relative stereochemistries were elucidated on the basis of spectroscopic data. This strategy is the first example of the gram-scale preparation of this series of compds. and presents a potential solution for increasing the gram-scale supply of novel natural products from marine sources.

IT **631913-68-3P**, Renieramycin O  
 RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);  
 PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study);  
 PREP (Preparation)  
 (oxidation product of renieramycin N)

RN 631913-68-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,7R,9R,14aS,15R)-7-cyano-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, (2Z)- (9CI) (CA INDEX NAME)

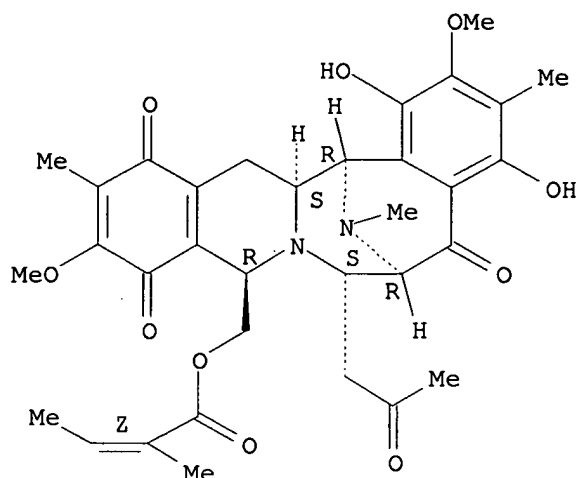
Absolute stereochemistry. Rotation (-).  
 Double bond geometry as shown.



IT **123641-95-2P**, Renieramycin E  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (renieramycin M transformation product)

RN 123641-95-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 7 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:585736 CAPLUS

DOCUMENT NUMBER: 139:227487

TITLE: Renieramycin J, a highly cytotoxic tetrahydroisoquinoline alkaloid, from a marine sponge *Neopetrosia* sp.

AUTHOR(S): Oku, Naoya; Matsunaga, Shigeki; Van Soest, Rob W. M.; Fusetani, Nobuhiro

CORPORATE SOURCE: Laboratory of Aquatic Natural Products Chemistry, Graduate School of Agricultural and Life Sciences, The University of Tokyo, Bunkyo, Tokyo, 113-8657, Japan

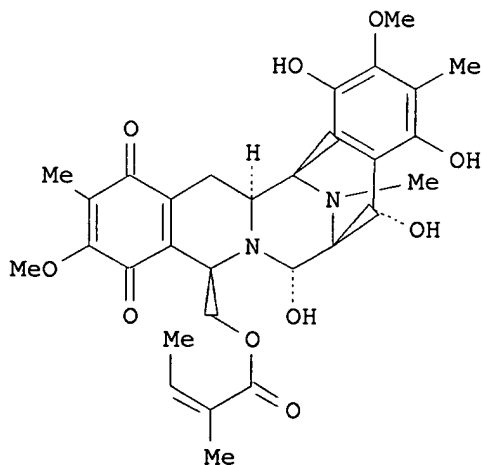
SOURCE: Journal of Natural Products (2003), 66(8), 1136-1139  
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

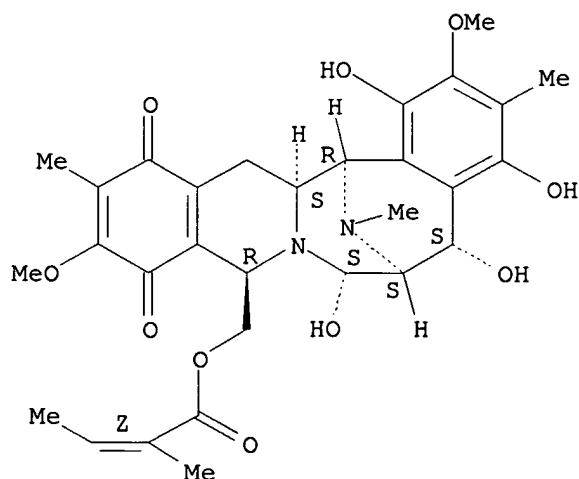
LANGUAGE: English

GI



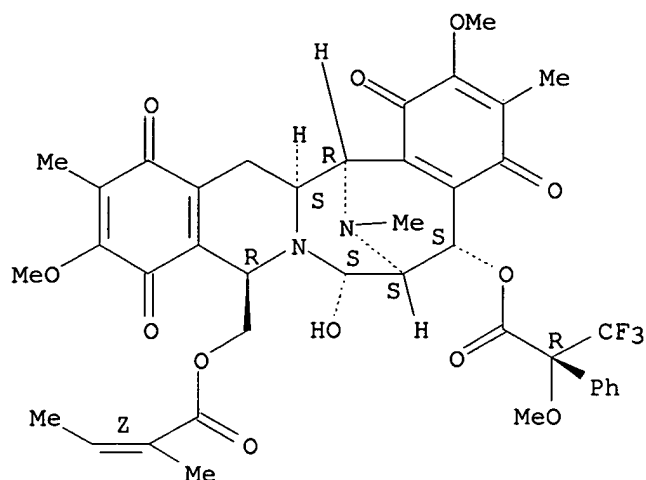
- AB Renieramycin J (I), a new tetrahydroisoquinoline alkaloid, has been isolated from a marine sponge *Neopetrosia* sp. as a potent cytotoxin that induced morphol. changes in 3Y1 cells. Such changes are characteristic of RNA and/or protein synthesis inhibitors. The structure of I including the absolute stereochem. was determined by spectroscopic and chemical methods.
- IT **593280-18-3P**, Renieramycin J (*Neopetrosia*)  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (cytotoxic tetrahydroisoquinoline alkaloid from marine sponge *Neopetrosia* sp.)
- RN 593280-18-3 CAPLUS
- CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-6,7,9,10,13,14,14a,15-octahydro-1,4,5,7-tetrahydroxy-2,11-dimethoxy-3,12,16-trimethyl-10,13-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).  
 Double bond geometry as shown.



- IT **592532-76-8P 592532-77-9P 592532-78-0P**  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and properties of)
- RN 592532-76-8 CAPLUS
- CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5,7-dihydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 8 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:955154 CAPLUS

DOCUMENT NUMBER: 138:205241

TITLE: Chemistry of renieramycins. Part 2. Partial reduction and nucleophilic substitution of hexahydro-1,5-imino-4-oxo-3-benzazocine-7,10-dione: Promising method to construct renieramycin J from renieramycin G via renieramycin E

AUTHOR(S): Koizumi, Yu-ichi; Kubo, Akinori; Suwanborirux, Khanit; Saito, Naoki

CORPORATE SOURCE: Meiji Pharmaceutical University, Tokyo, 204-8588, Japan

SOURCE: Heterocycles (2002), 57(12), 2345-2355

CODEN: HTCYAM; ISSN: 0385-5414

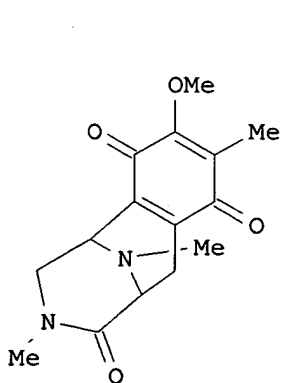
PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal

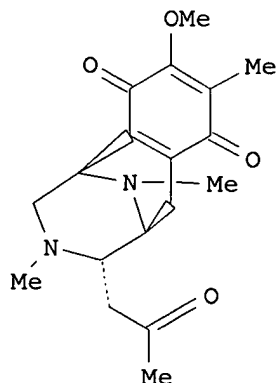
LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:205241

GI



I



II

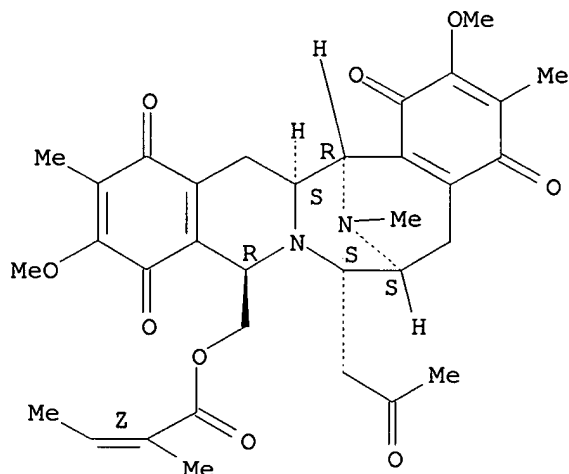
AB The conversion of 1,2,3,4,5,6,7,10-octahydro-9-methoxy-3,8,11-trimethyl-1,5-imino-3-benzazocine-4,7,10-trione (I) to the corresponding alkylated compound at C-21 position, II, as an ABC ring model of renieramycin J is described. This is a promising method for converting renieramycin G into renieramycin J via renieramycin E. The antitumor activity of some of the prepared compds. was evaluated in several cancer cell lines.

IT **500111-59-1P**, Renieramycin J  
 RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (preparation of an ABC ring model of renieramycin J from a lactam carbonyl via partial reduction and nucleophilic substitution)

RN 500111-59-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-7-(2-oxopropyl)-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
 Double bond geometry as shown.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 9 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:765217 CAPLUS

DOCUMENT NUMBER: 138:14135

TITLE: A Solid-Supported, Enantioselective Synthesis Suitable for the Rapid Preparation of Large Numbers of Diverse Structural Analogues of (-)-Saframycin A

AUTHOR(S): Myers, Andrew G.; Lanman, Brian A.

CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA

SOURCE: Journal of the American Chemical Society (2002), 124(44), 12969-12971  
 CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

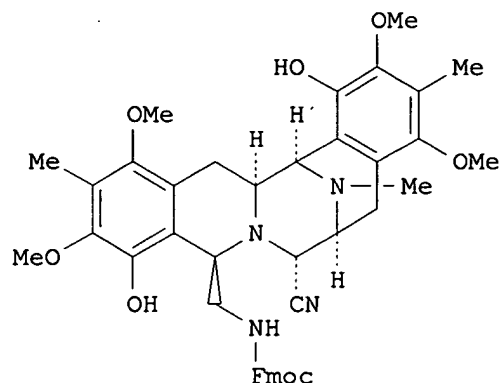
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:14135

GI





AB A 10-step solid-supported, enantioselective synthesis suitable for the rapid preparation of large nos. of diverse structural analogs of saframycin A is described. The synthetic route, which bears analogy to solid-phase peptide synthesis, involves the directed condensation of N-protected  $\alpha$ -amino aldehyde reactants, e.g. N-Fmoc-glycinal (Fmoc = 9-fluorenylmethoxycarbonyl). A novel dual linker, (S)-2-[4-(tert-butyl)dimethylsilyloxy]-1-butyl]morpholine, was developed for attachment of intermediates to the solid support via a C-protective group, a substituted morpholino nitrile derivative. The route employs a novel diastereospecific cyclorelease mechanism, supports structural variation at multiple sites in the saframycin core, and obviates the need for chromatog. purification of the products or any intermediate. To demonstrate the feasibility of structural variation at multiple sites, a matrix of 16 saframycin A analogs, e.g. I, was prepared by parallel synthesis with simultaneous variation of two sites. This work is notable not only as a preliminary step toward large-scale library construction but also as an example of the use of sequential stereoselective C-C bond-forming reactions on the solid phase for the preparation of natural product analogs.

IT **429687-39-8P 477566-41-9P 477566-42-0P**  
**477566-43-1P 477566-44-2P 477566-56-6P**  
**477566-57-7P**

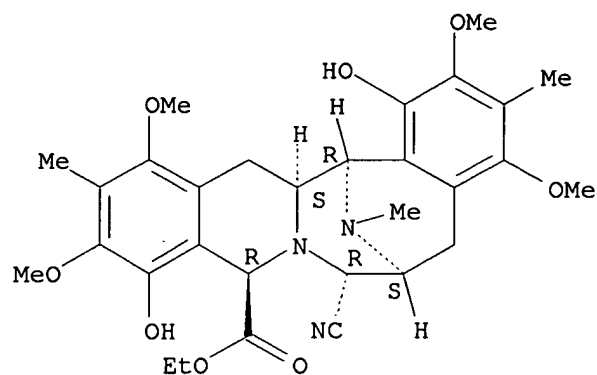
RL: SPN (Synthetic preparation); PREP (Preparation)  
 (asym. synthesis of (-)-saframycin A analogs via solid-supported combinatorial chemical using a directed condensation of N-protected amino aldehydes with (silyloxybutyl)morpholine dual linker and Pictet-Spengler cyclization)

RN 429687-39-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
 7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-  
 3,12,16-trimethyl-, ethyl ester, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX  
 NAME)

Absolute stereochemistry.

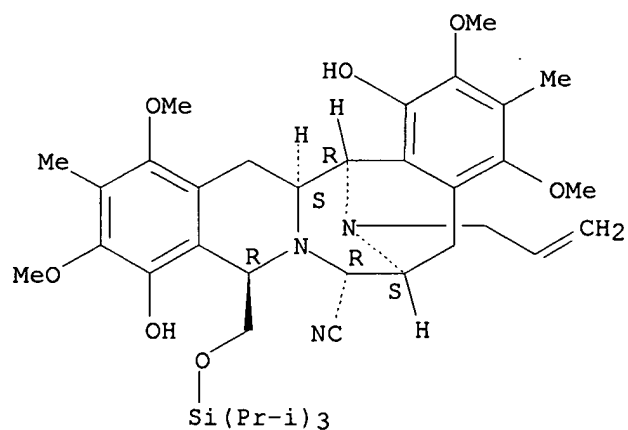
10/826,859



RN 477566-41-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,  
6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12-  
dimethyl-16-(2-propenyl)-9-[[[tris(1-methylethyl)silyl]oxy]methyl]-,  
(6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

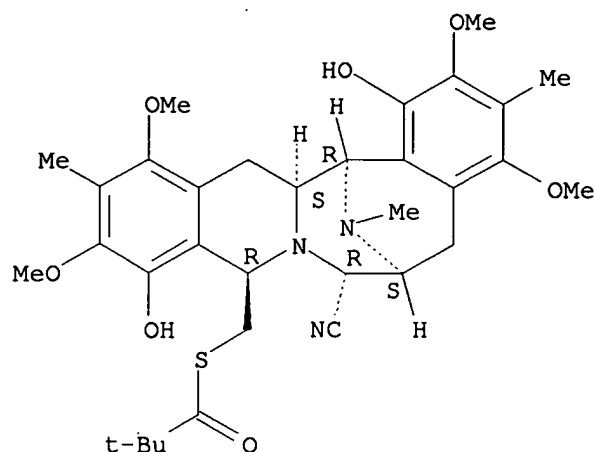
Absolute stereochemistry.



RN 477566-42-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7-carbonitrile,  
6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12-  
dimethyl-16-(2-propynyl)-9-[[[tris(1-methylethyl)silyl]oxy]methyl]-,  
(6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 10 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:391711 CAPLUS

DOCUMENT NUMBER: 136:401914

TITLE: Preparation of saframycin analogs for pharmaceutical use in the treatment of cancer

INVENTOR(S): Myers, Andrew; Plowright, Alleyn T.; Kung, Daniel W.; Lanman, Brian; Barbay, Joseph; Xing, Chengguo

PATENT ASSIGNEE(S): President and Fellows of Harvard College, USA

SOURCE: PCT Int. Appl., 203 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

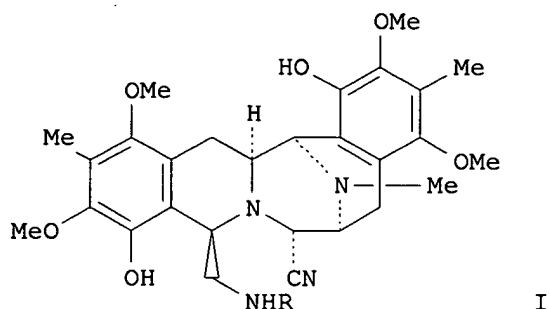
*Parent*

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040477	A2	20020523	WO 2001-US47399	20011105
WO 2002040477	A3	20030227		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002039565	A5	20020527	AU 2002-39565	20011105
US 2003008873	A1	20030109	US 2001-11466	20011105
US 6809099	B2	20041026		
EP 1339713	A2	20030903	EP 2001-987338	20011105
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004529074	T2	20040924	JP 2002-543487	20011105
US 2004204419	A1	20041014	US 2004-826859	20040416
PRIORITY APPLN. INFO.:				
			US 2000-245888P	P 20001103
			US 2001-11466	A3 20011105
			WO 2001-US47399	W 20011105

10/826,859

OTHER SOURCE(S):  
GI

MARPAT 136:401914



AB Saframycin analogs, such as I [R = H, alkyl, acyl, arylacyl, heteroarylacyl, carboxy, arylsulfonyl, etc.], were prepared for therapeutic use as antitumor agents. Thus, I (R = 2-furanylmethyl) was prepared in 95% yield via condensation of 2-furancarboxaldehyde with the corresponding amine I (R = NH<sub>2</sub>) using sodium triacetoxyborohydride in MeCN. The amine I (R = H) was prepared via a stereoselective sequence of solid phase synthetic steps. The prepared saframycin analogs were assayed for cancer cell growth inhibition of A375 malignant melanoma and A-459 lung carcinoma cell lines.

IT **429687-39-8P**

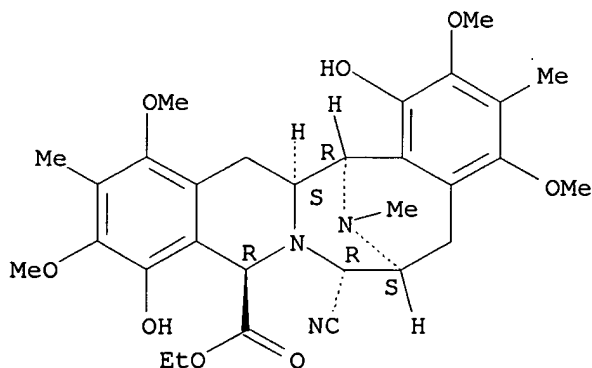
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of saframycin analogs for pharmaceutical use in the treatment of cancer)

RN 429687-39-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 7-cyano-6,7,9,14,14a,15-hexahydro-1,10-dihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-, ethyl ester, (6S,7R,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 11 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:545697 CAPLUS

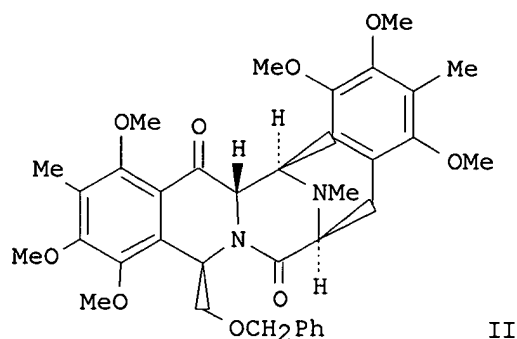
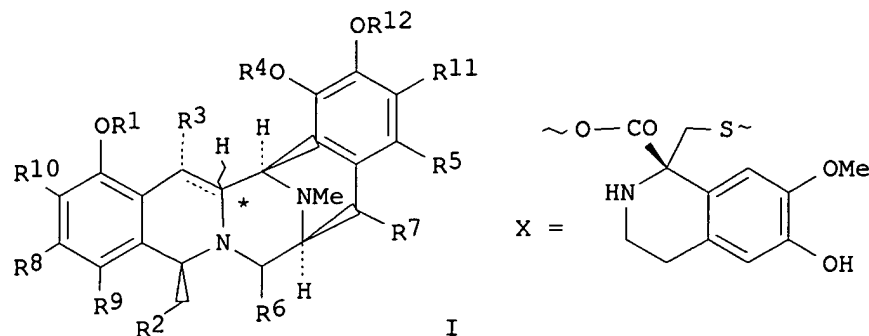
DOCUMENT NUMBER: 135:137633

TITLE: Preparation of saframycin-ecteinascidin analogs and

10/826,859

INVENTOR(S): their therapeutic applications  
PATENT ASSIGNEE(S): Danishefsky, Samuel J.; Zhou, Bishan  
SOURCE: The Trustees of Columbia University in the City of New  
York, USA  
DOCUMENT TYPE: PCT Int. Appl., 115 pp.  
LANGUAGE: CODEN: PIXXD2  
FAMILY ACC. NUM. COUNT: Patent  
PATENT INFORMATION: English  
1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053299	A1	20010726	WO 2001-US1877	20010119
WO 2001053299	C2	20021024		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2397597	AA	20010726	CA 2001-2397597	20010119
US 2002025962	A1	20020228	US 2001-765515	20010119
US 6686470	B2	20040203		
EP 1254140	A1	20021106	EP 2001-903151	20010119
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2003520801	T2	20030708	JP 2001-553773	20010119
US 2004127709	A1	20040701	US 2003-728580	20031205
PRIORITY APPLN. INFO.:			US 2000-177071P	P 20000119
			US 2001-765515	A3 20010119
			WO 2001-US1877	W 20010119
OTHER SOURCE(S):	MARPAT 135:137633			
GI				



AB Compds. of the saframycin-ecteinascidin series such as I [R1,R4 = H, alkyl, acyl; R3 = =O, OH, ether, sulfide, acyl group such as OC(O)Me, OC(O)Bn and OC(O)Et; R5 = H, halogen, OH, ether, acyl, amide; R6 = =O, OH, OMe, CN, acyloxy; R7 = =O, OH, halogen, ether, acyl; R8 and R9 independently = H, Me, OMe, OEt, CF3, Br, F; R8R9 = OCH2O, five or six membered ring; R10,R11 = Me, OMe, OEt, SMe, SET; R12 = H, alkyl, acyl; chiral center marked \* has the R or the S configuration], were prepared for use as antitumor and antimicrobial agents. Thus, saframycin analog II was prepared via a multistep synthetic sequence starting from 2,4-Dimethoxy-3-methylbenzaldehyde, bromoacetal, 2-hydroxy-4-methoxy-3-methylbenzaldehyde and [(2E)-4-bromo-2-butenyl]oxy(1,1-dimethylethyl)dimethylsilane. Ecteinascidin 743 I (R1 = Ac, R2R3 = X, R4 = R5 = R7 = H, R6 =  $\alpha$ -OH, R8R9 = OCH2O, R10-R12 = Me) was tested for cytotoxicity and antimicrobial activity.

IT **351378-59-1P 351378-84-2P 351378-93-3P**

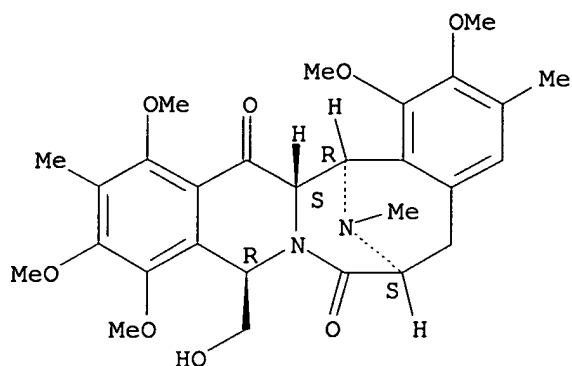
RL: PNU (Preparation, unclassified); PREP (Preparation)  
(attempted synthesis of)

RN 351378-59-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-9-(hydroxymethyl)-1,2,10,11,13-pentamethoxy-3,12,16-  
trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

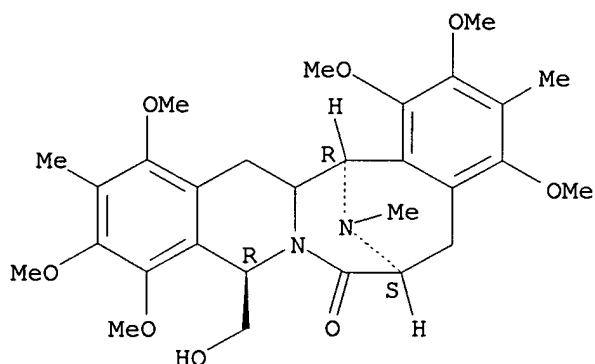
10/826,859



RN 351378-84-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

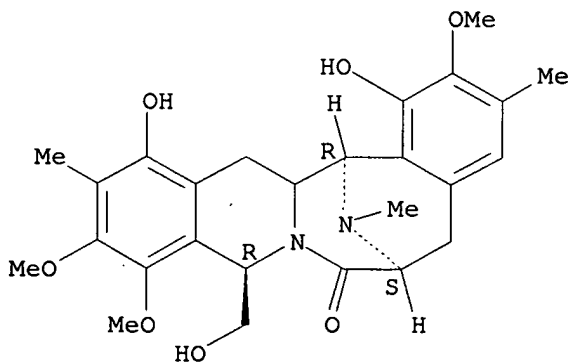
Absolute stereochemistry.



RN 351378-93-3 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 351377-83-8P 351377-84-9P 351377-85-0P

351377-86-1P 351377-88-3P 351378-45-5P

351379-85-6P 351379-86-7P 351379-88-9P

351379-89-0P

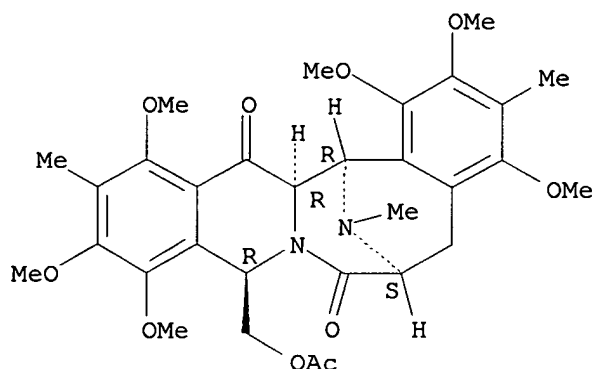
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of saframycin-ec-teinascidin analogs and their therapeutic applications)

RN 351377-83-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(acetyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

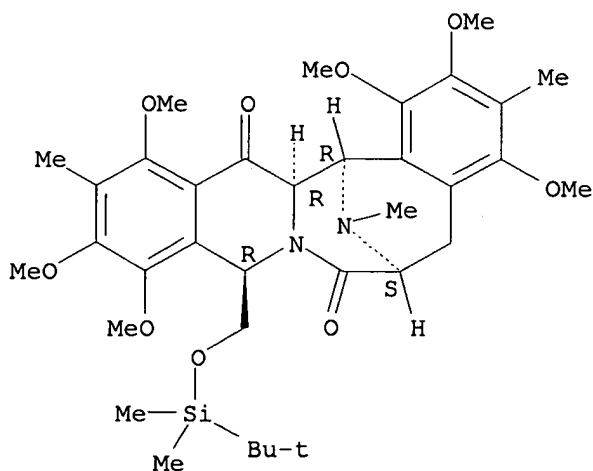
Absolute stereochemistry.



RN 351377-84-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 351377-85-0 CAPLUS

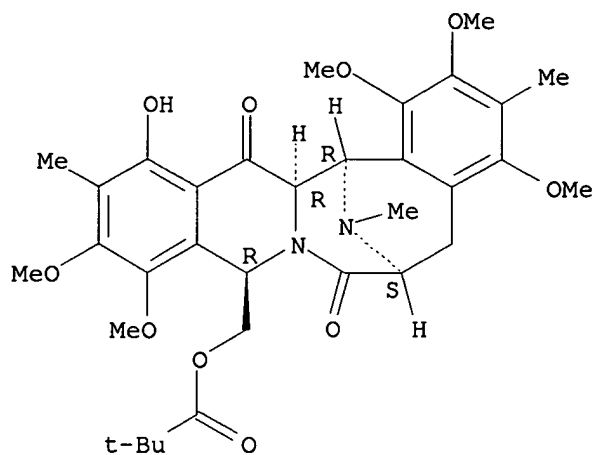
CN Propanoic acid, 2,2-dimethyl-, [(6S,9R,14aR,15R)-6,7,9,14,14a,15-hexahydro-13-hydroxy-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-7,14-dioxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester (9CI) (CA INDEX NAME)



10/826,859

NAME)

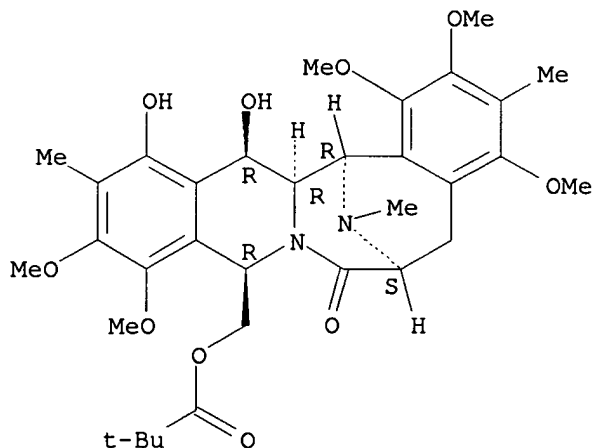
Absolute stereochemistry.



RN 351377-86-1 CAPLUS

CN Propanoic acid, 2,2-dimethyl-, [(6S,9R,14R,14aR,15R)-6,7,9,14,14a,15-hexahydro-13,14-dihydroxy-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-7-oxo-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

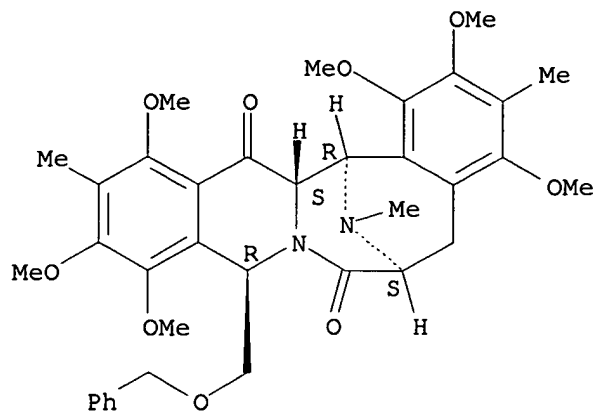


RN 351377-88-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

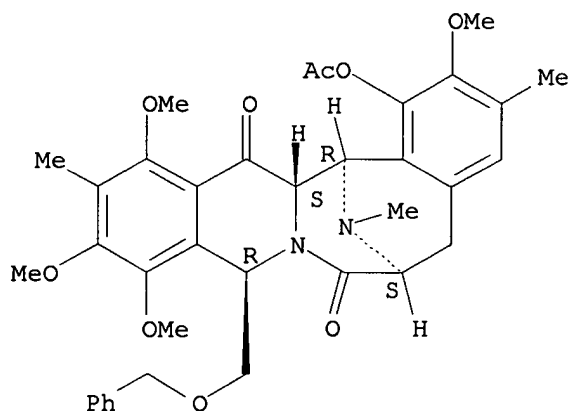
10/826,859



RN 351378-45-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
1-(acetyloxy)-14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

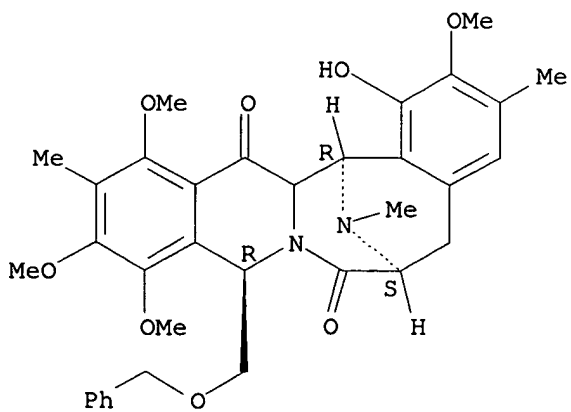
Absolute stereochemistry.



RN 351379-85-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

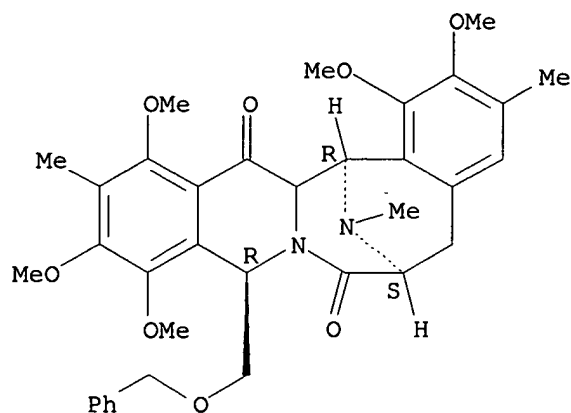


10/826,859

RN 351379-86-7 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

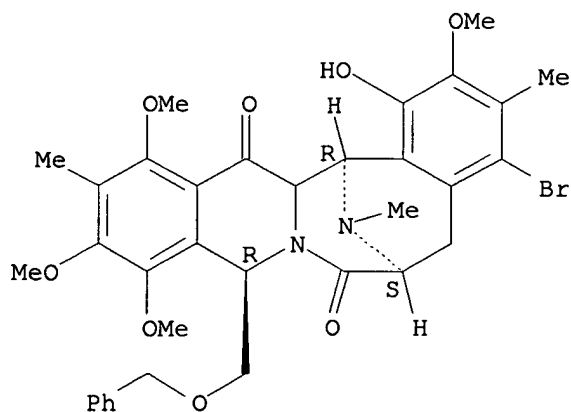
Absolute stereochemistry.



RN 351379-88-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
4-bromo-14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

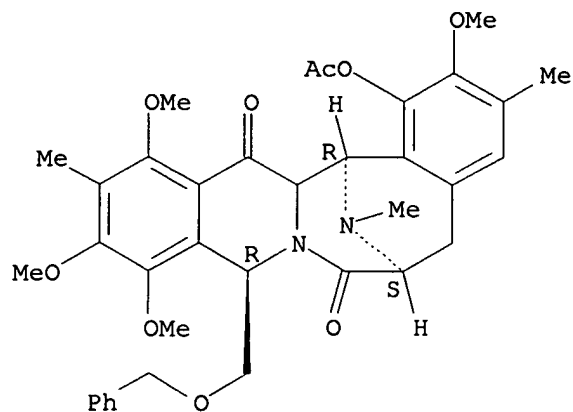
Absolute stereochemistry.



RN 351379-89-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
1-(acetyloxy)-14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



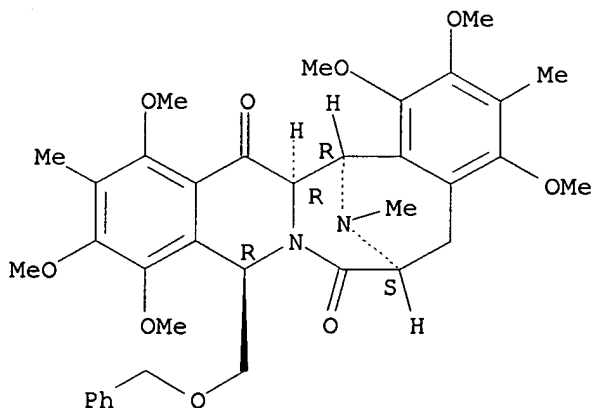
IT 271578-62-2P 273720-76-6P 351377-77-0P  
 351377-78-1P 351377-79-2P 351377-81-6P  
 351378-24-0P 351378-26-2P 351378-28-4P  
 351378-30-8P 351378-32-0P 351378-43-3P  
 351378-57-9P 351378-78-4P 351379-71-0P  
 351379-73-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of saframycin-ecteinascidin analogs and their therapeutic  
 applications)

RN 271578-62-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-  
 [(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

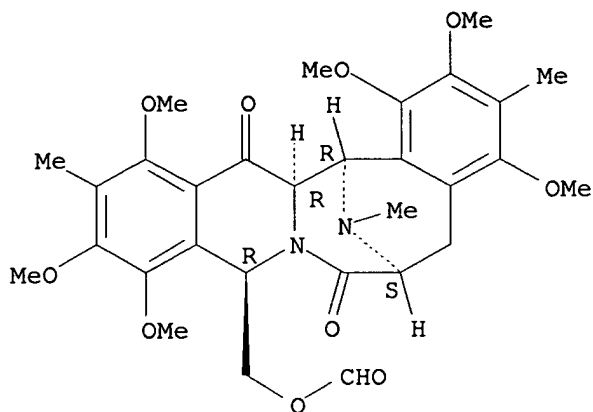


RN 273720-76-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
 9-[(formyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-  
 trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

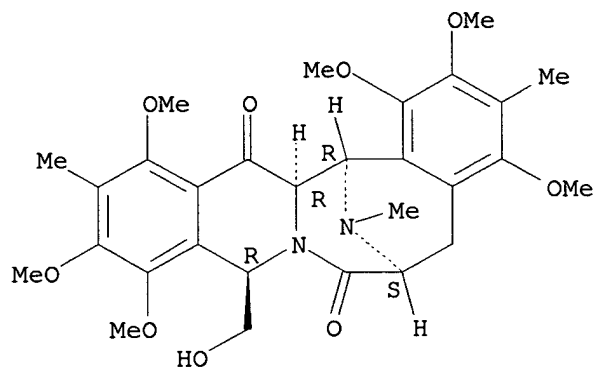
10/826,859



RN 351377-77-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-  
trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

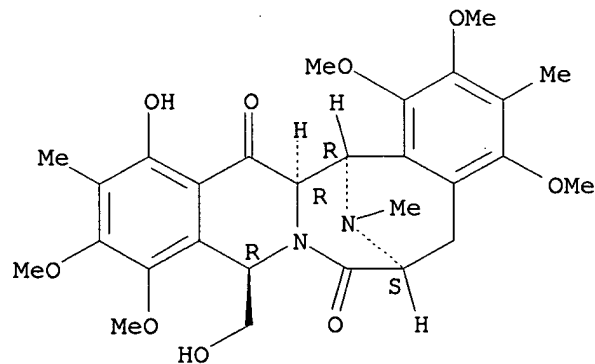
Absolute stereochemistry.



RN 351377-78-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-  
3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

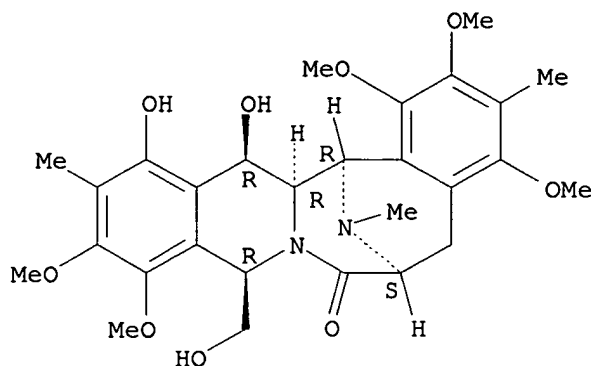


10/826,859

RN 351377-79-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-13,14-dihydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-trimethyl-, (6S,9R,14R,14aR,15R)- (9CI) (CA INDEX NAME)

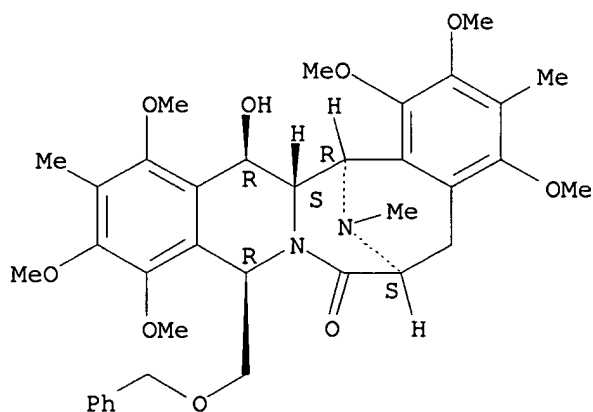
Absolute stereochemistry.



RN 351377-81-6 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-14-hydroxy-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

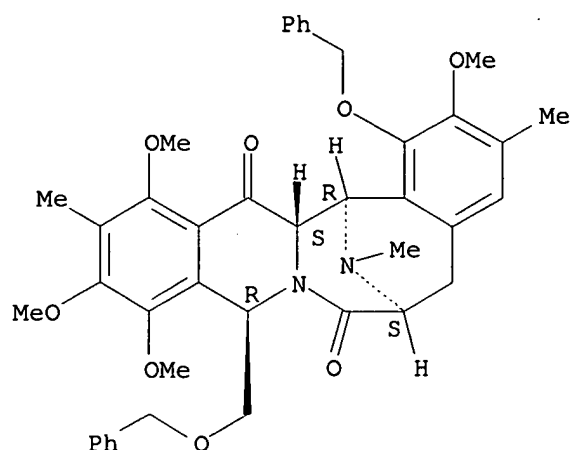


RN 351378-24-0 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-1-(phenylmethoxy)-9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

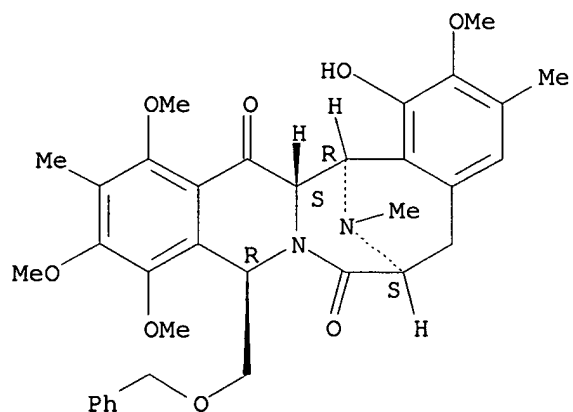
10/826,859



RN 351378-26-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

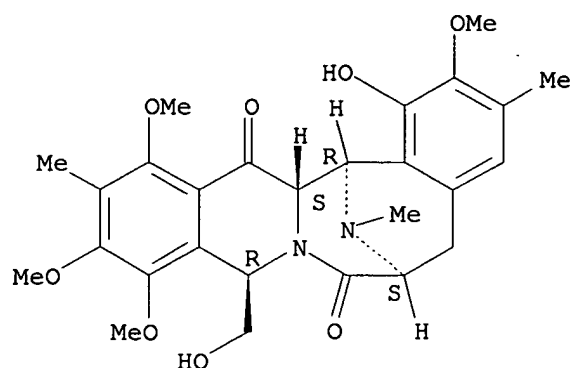


RN 351378-28-4 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-1-hydroxy-9-(hydroxymethyl)-2,10,11,13-tetramethoxy-3,12,16-  
trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

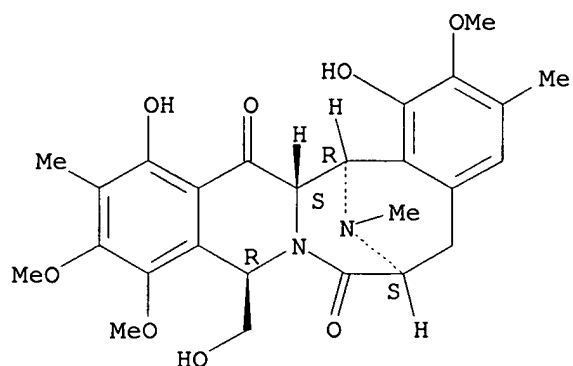
10/826,859



RN 351378-30-8 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-1,13-dihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-  
trimethyl-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

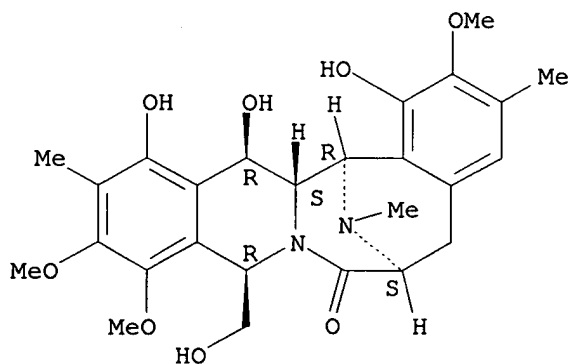
Absolute stereochemistry.



RN 351378-32-0 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-  
hexahydro-1,13,14-trihydroxy-9-(hydroxymethyl)-2,10,11-trimethoxy-3,12,16-  
trimethyl-, (6S,9R,14R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



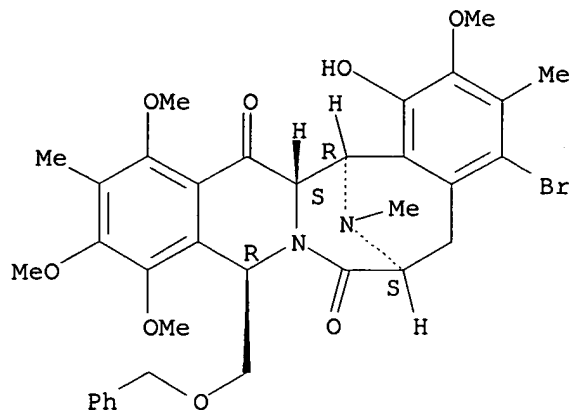
RN 351378-43-3 CAPLUS



10/826,859

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
4-bromo-14a,15-dihydro-1-hydroxy-2,10,11,13-tetramethoxy-3,12,16-trimethyl-  
9-[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

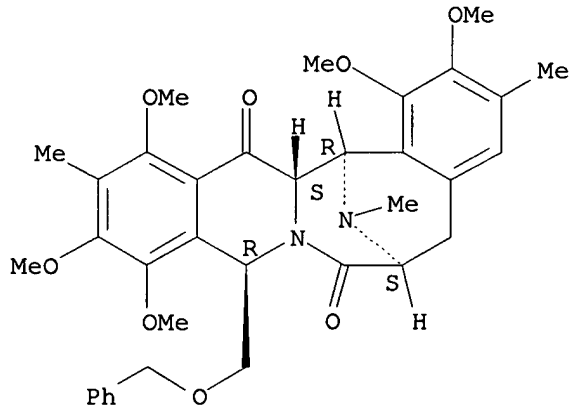
Absolute stereochemistry.



RN 351378-57-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,  
14a,15-dihydro-1,2,10,11,13-pentamethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

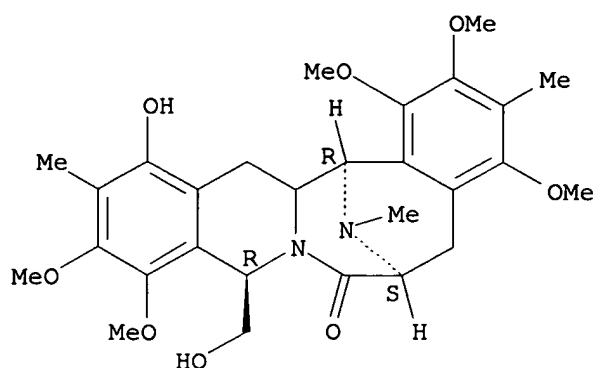


RN 351378-78-4 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-  
hexahydro-13-hydroxy-9-(hydroxymethyl)-1,2,4,10,11-pentamethoxy-3,12,16-  
trimethyl-, (6S,9R,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

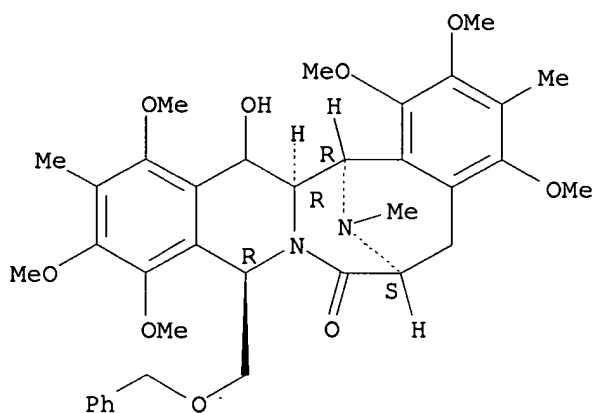
10/826,859



RN 351379-71-0 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-14-hydroxy-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)-(9CI) (CA INDEX NAME)

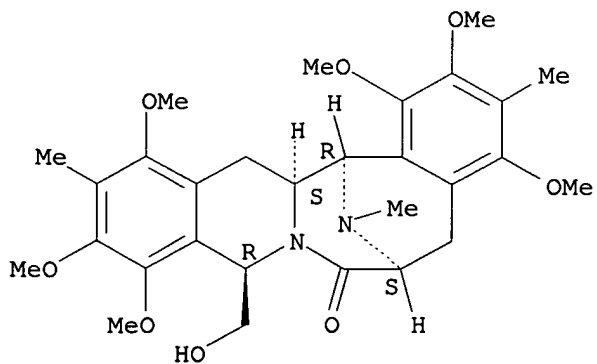
Absolute stereochemistry.



RN 351379-73-2 CAPLUS

CN 6,15-Imino-7H-isoquino[3,2-b][3]benzazocin-7-one, 5,6,9,14,14a,15-hexahydro-9-(hydroxymethyl)-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aS,15R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



10/826,859

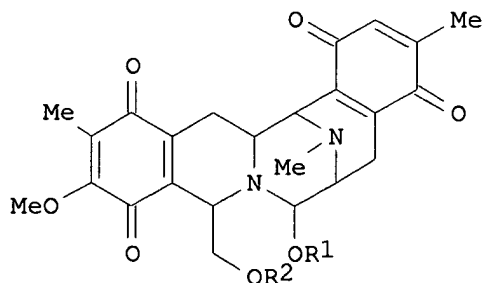
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 12 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2001:208273 CAPLUS  
DOCUMENT NUMBER: 134:219960  
TITLE: New antitumor marine alkaloids  
INVENTOR(S): Cimino, Guido; Fontana, Angelo; Garcia Gravalos, Dolores; Wahidulla, Solimabi  
PATENT ASSIGNEE(S): Instituto Biomar, S.A., Spain; Ruffles, Graham Keith  
SOURCE: PCT Int. Appl., 9 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

1449

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001019824	A2	20010322	WO 2000-GB3489	20000911
WO 2001019824	A3	20010927		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
CA 2384656	AA	20010322	CA 2000-2384656	20000911
AU 2000070285	A5	20010417	AU 2000-70285	20000911
BR 2000014176	A	20020507	BR 2000-14176	20000911
EP 1210346	A2	20020605	EP 2000-958872	20000911
EP 1210346	B1	20030702		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
JP 2003509424	T2	20030311	JP 2001-523401	20000911
AT 244242	E	20030715	AT 2000-958872	20000911
PT 1210346	T	20030930	PT 2000-958872	20000911
ES 2200922	T3	20040316	ES 2000-958872	20000911
PRIORITY APPLN. INFO.:			GB 1999-21477	A 19990910
			WO 2000-GB3489	W 20000911

OTHER SOURCE(S): MARPAT 134:219960  
GI



I

AB New antitumor alkaloids I (R1 = H, alkyl or acyl; R2 = H or acyl), which include jorumycin (I, R1 = H, R2 = acetyl), were extracted from the mollusc *Jorunna funebris*. The antitumor IC50 of jorumycin against P-388 tumor cells was 0.02  $\mu$ M and it was also active against gram-pos. bacteria (no data).

IT **304852-37-7P**, Jorumycin

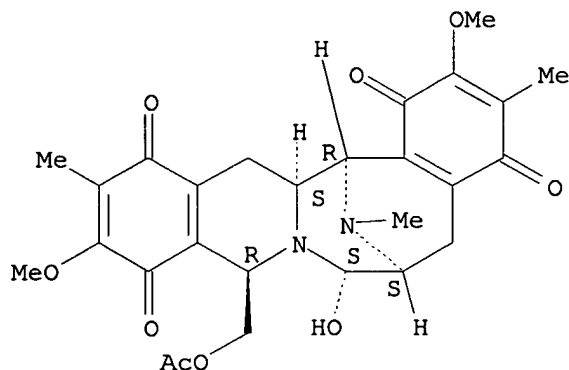
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(jorumycin antitumor alkaloid from *Jorunna funebris*)

RN 304852-37-7 CAPLUS

CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(5H)-tetrone, 9-[(acetyloxy)methyl]-6,7,9,14,14a,15-hexahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-, (6S,7S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L7 ANSWER 13 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:645105 CAPLUS

DOCUMENT NUMBER: 133:347376

TITLE: A new antitumor isoquinoline alkaloid from the marine nudibranch *Jorunna funebris*

AUTHOR(S): Fontana, A.; Cavaliere, P.; Wahidulla, S.; Naik, C. G.; Cimino, G.

CORPORATE SOURCE: Istituto per la Chimica di Molecole di Interesse Biologico (ICMIB) del CNR, Arco Felice (Na), 80072, Italy

SOURCE: Tetrahedron (2000), 56(37), 7305-7308

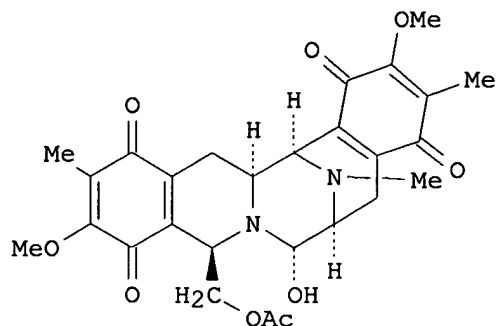
CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB A new dimeric isoquinoline alkaloid, jorumycin (I), has been isolated from the skin and the mucus of the Pacific nudibranch *Jorunna funebris*. The structure has been fully elucidated on the grounds of ESMS data and of an extensive 2D NMR anal. The cytotoxicity of I was evaluated against various human cancer cell lines and was found to be slightly less potent than Et 743.

IT 304852-37-7P, Jorumycine

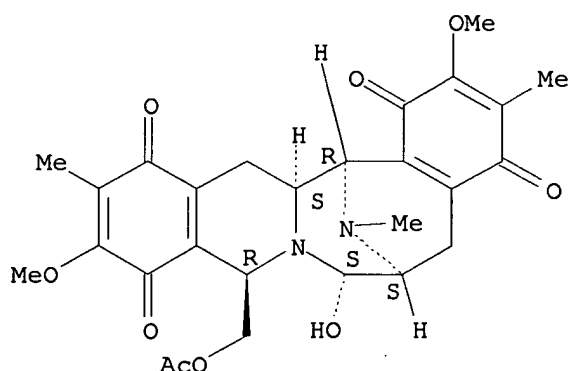
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(antitumor isoquinoline alkaloid from marine nudibranch *Jorunna funebris*)

RN 304852-37-7 CAPLUS

CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(5H)-tetrone, 9-[(acetyloxy)methyl]-6,7,9,14,14a,15-hexahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-, (6S,7S,9R,14aS,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 14 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:248566 CAPLUS

DOCUMENT NUMBER: 133:30850

TITLE: A novel face specific Mannich closure providing access to the saframycin-ecteinascidin series of piperazine based alkaloids

AUTHOR(S): Zhou, Bishan; Guo, Jinsong; Danishefsky, Samuel J.

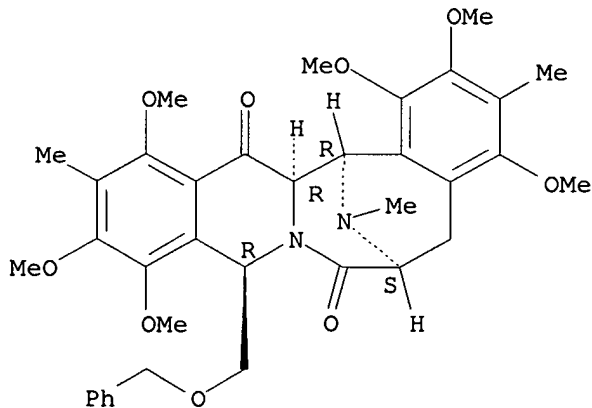
CORPORATE SOURCE: The Department of Chemistry, Columbia University, New

SOURCE: York, NY, 10027, USA  
 Tetrahedron Letters (2000), 41(13), 2043-2046  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 133:30850  
 GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

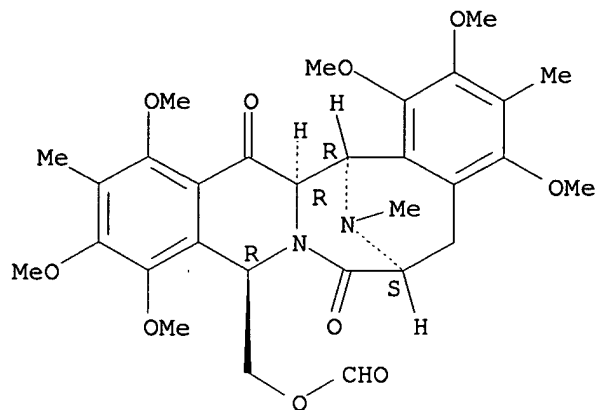
AB The Mannich-like closure of I to II directly provides the backbone stereochem. required for the titled alkaloids, in contrast to the stereochem. outcome in a related earlier case.  
 IT **271578-62-2P**  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (face specific Mannich closure providing access to saframycin-ecteinascidin series of piperazine based alkaloids)  
 RN 271578-62-2 CAPLUS  
 CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **273720-76-6P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (face specific Mannich closure providing access to saframycin-ecteinascidin series of piperazine based alkaloids)  
 RN 273720-76-6 CAPLUS  
 CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione, 9-[(formyloxy)methyl]-14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 15 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:248565 CAPLUS

DOCUMENT NUMBER: 133:4840

TITLE: Synthetic explorations in the saframycin-ecteinascidin series: construction of major chiral subunits through catalytic asymmetric induction

AUTHOR(S): Zhou, Bishan; Edmondson, Scott; Padron, Juan; Danishefsky, Samuel J.

CORPORATE SOURCE: The Department of Chemistry, Columbia University, New York, NY, 10027, USA

SOURCE: Tetrahedron Letters (2000), 41(13), 2039-2042

CODEN: TELEAY; ISSN: 0040-4039

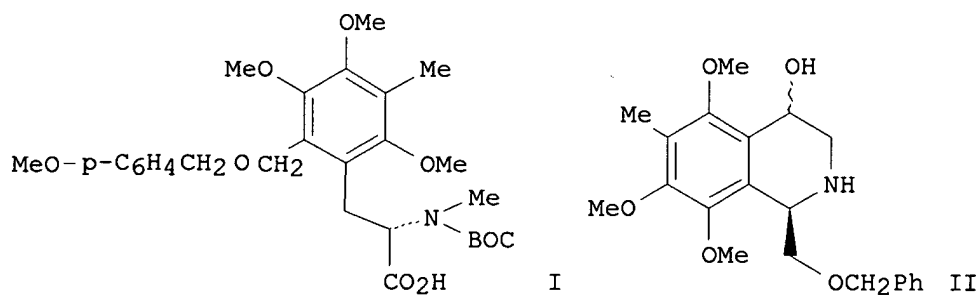
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:4840

GI



AB The major subunits (I and II) needed to reach the titled targets have been assembled by chemical, which included p-Claisen rearrangement, asym. epoxidn. and asym. dihydroxylation.

IT **271578-62-2P**

RL: PNU (Preparation, unclassified); PREP (Preparation)  
(construction of major chiral saframycin subunits via catalytic asym. induction)

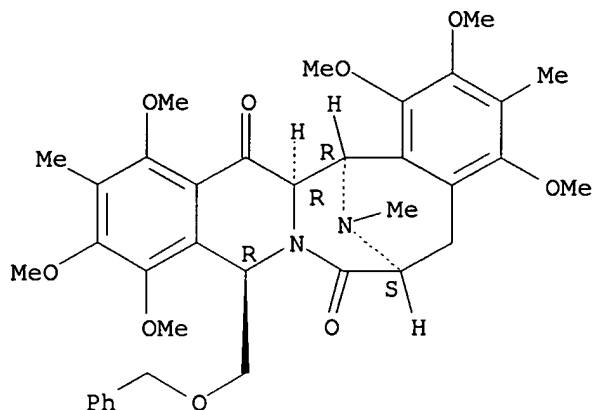
RN 271578-62-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-7,14(6H,9H)-dione,

10/826,859

14a,15-dihydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-9-  
[(phenylmethoxy)methyl]-, (6S,9R,14aR,15R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 16 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:717839 CAPLUS

DOCUMENT NUMBER: 123:227861

TITLE: Synthesis of saframycins. XI. Synthetic studies toward  
a total synthesis of safracin A

AUTHOR(S): Saito, Naoki; Harada, Shunji; Yamashita, Mihoko;  
Saito, Takeshi; Yamaguchi, Kentaro; Kubo, Akinori

CORPORATE SOURCE: Meiji Coll. Pharmacy, Tokyo, 154, Japan

SOURCE: Tetrahedron (1995), 51(30), 8213-30

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Pergamon

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:227861

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A synthetic strategy for the preparation of the isoquinolinequinone antibiotic safracin A is outlined. The authors' initial strategy for the construction of the ABC ring was based on a retrosynthetic anal. Conversion of piperazinedione I in five steps to the imide was followed by a 1,2-reduction with lithium tri-tert-butoxyaluminum hydride to give the allylic alc. II. This compound was then cyclized to the 1,5-imino-3-benzazocine III (R = CO<sub>2</sub>CHMe<sub>2</sub>) and an unwanted indeno[1,2-b]pyrazin-2-one. Conversion of III (R = H) to the pentacyclic pyruvamide IV was completed in a nine step sequence. Finally, IV was subjected to a two-step oxidative demethylation to provide the quinones V (R<sub>1</sub> = Me, R<sub>2</sub> = H; R<sub>1</sub> = H, R<sub>2</sub> = NO<sub>2</sub>). An unsuccessful attempt to introduce a hydroxyl group into the C-1 position of the quinones V is also described.

IT 168132-84-1P 168132-86-3P 168254-07-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT



10/826,859

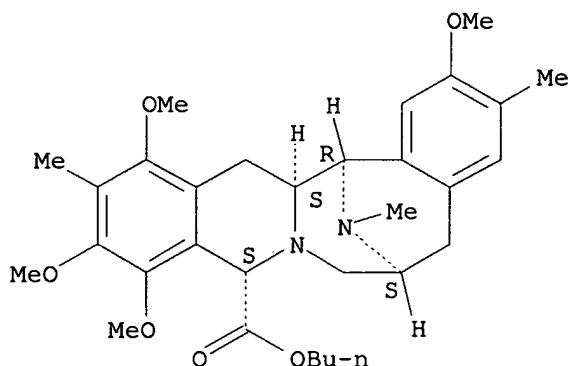
(Reactant or reagent)

(synthetic studies toward total synthesis of safracin A)

RN 168132-84-1 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-,  
butyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

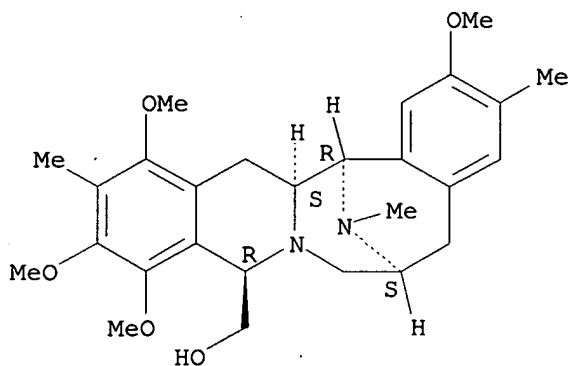
Relative stereochemistry.



RN 168132-86-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\beta$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.

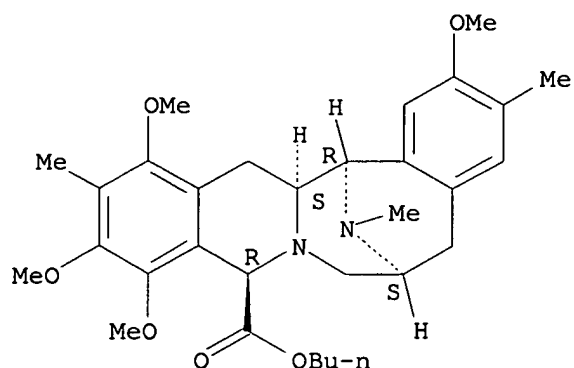


RN 168254-07-7 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-2,10,11,13-tetramethoxy-3,12,16-trimethyl-,  
butyl ester, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.

10/826,859



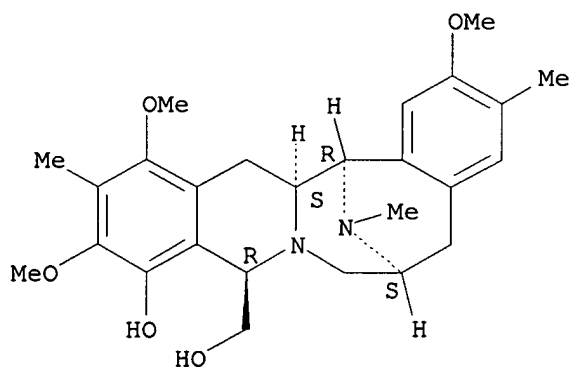
IT 168132-87-4P 168132-88-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthetic studies toward total synthesis of safracin A)

RN 168132-87-4 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-10-hydroxy-2,11,13-trimethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

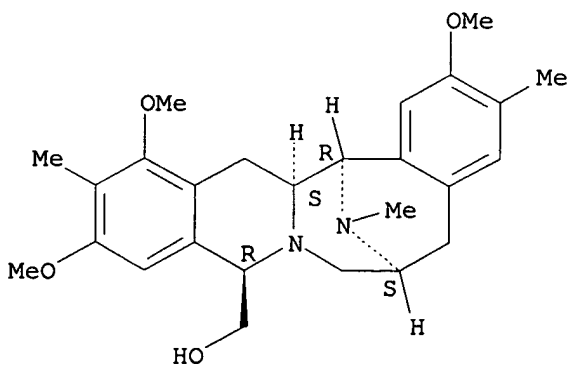
Relative stereochemistry.



RN 168132-88-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-2,11,13-trimethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

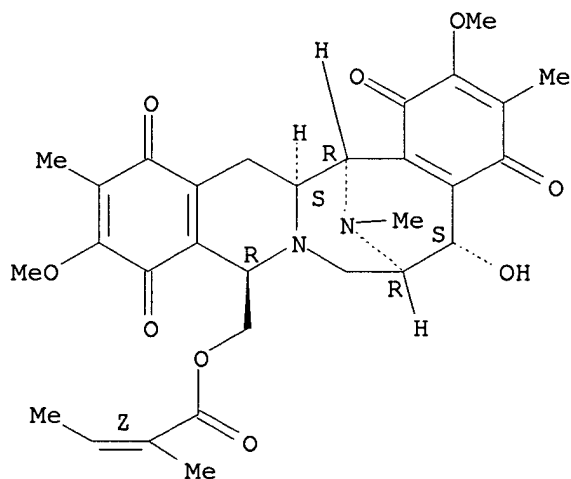
Relative stereochemistry.



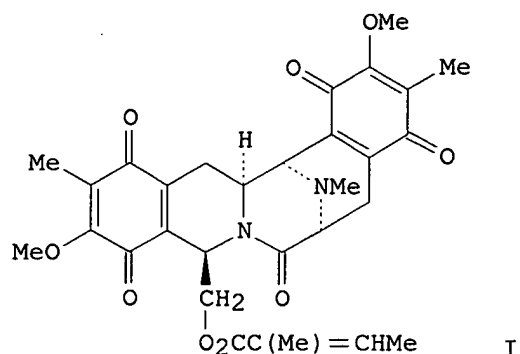
10/826,859

L7 ANSWER 17 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1994:298315 CAPLUS  
DOCUMENT NUMBER: 120:298315  
TITLE: A stereocontrolled total synthesis of  
(±)-renieramycin A  
AUTHOR(S): Linton, Steven Douglas  
CORPORATE SOURCE: Rice Univ., Houston, TX, USA  
SOURCE: (1992) 149 pp. Avail.: Univ. Microfilms Int., Order  
No. DA9234382  
From: Diss. Abstr. Int. B 1993, 53(7), 3485  
DOCUMENT TYPE: Dissertation  
LANGUAGE: English  
AB Unavailable  
IT **132342-06-4P**, (±)-Renieramycin A  
RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(stereocontrolled total synthesis of)  
RN 132342-06-4 CAPLUS  
CN 2-Butenoic acid, 2-methyl-, (1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-  
2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-  
isoquino[3,2-b][3]benzazocin-9-yl)methyl ester,  
[5α,6α,9β(Z),14aa,15α]- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.  
Double bond geometry as shown.



1449  
L7 ANSWER 18 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1992:547449 CAPLUS  
DOCUMENT NUMBER: 117:147449  
TITLE: Renieramycin G, a new alkaloid from the sponge  
Xestospongia caycedoi  
AUTHOR(S): Davidson, Bradley S.  
CORPORATE SOURCE: Dep. Chem., Univ. Hawaii, Honolulu, HI, 96822, USA  
SOURCE: Tetrahedron Letters (1992), 33(26), 3721-4  
CODEN: TELEAY; ISSN: 0040-4039  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB A new cytotoxic alkaloid, renieramycin G (I), was isolated, along with previously reported metabolites mimosamycin, renierol, and N-formyl-1,2-dihydrorenierone, from the Fijian sponge *X. caycedoi*. The structure of renieramycin G was deduced from spectral data.

IT **143458-75-7**, Renieramycin G

RL: BIOL (Biological study)

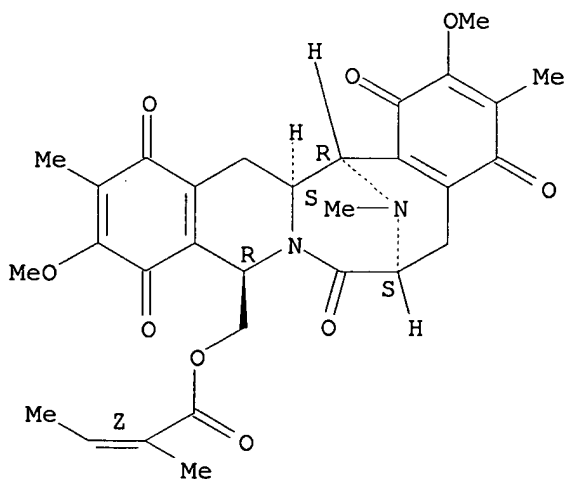
(from *Xestospongia caycedoi*, structure of)

RN 143458-75-7 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6S-[6 $\alpha$ ,9 $\beta$ (Z),14 $\alpha$ ,15 $\alpha$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



L7 ANSWER 19 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

1449  
ACCESSION NUMBER: 1991:608305 CAPLUS

DOCUMENT NUMBER: 115:208305

TITLE: Synthesis of saframycins. VII. The synthesis of novel renieramycin congeners

AUTHOR(S): Saito, Naoki; Yamauchi, Reiko; Kubo, Akinori

CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan

SOURCE: Heterocycles (1991), 32(6), 1203-14

DOCUMENT TYPE:

Journal

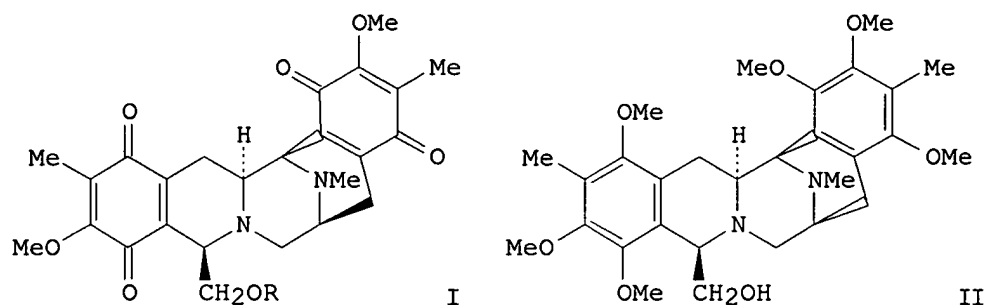
LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 115:208305

GI



AB The marine alkaloid renieramycin congeners I (R = H, Ac, EtCO) were synthesized starting from the alc. II which was the key intermediate for saframycin B synthesis.

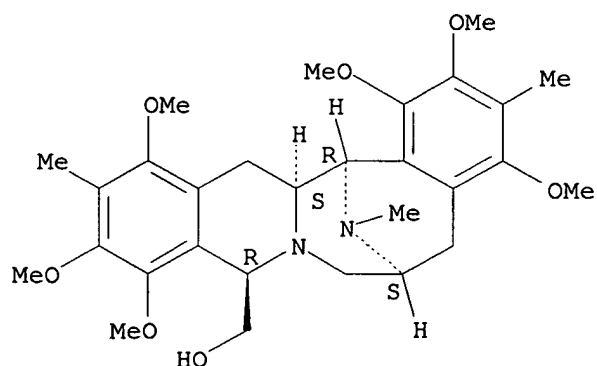
IT 112446-04-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 112995-91-2P 136581-76-5P

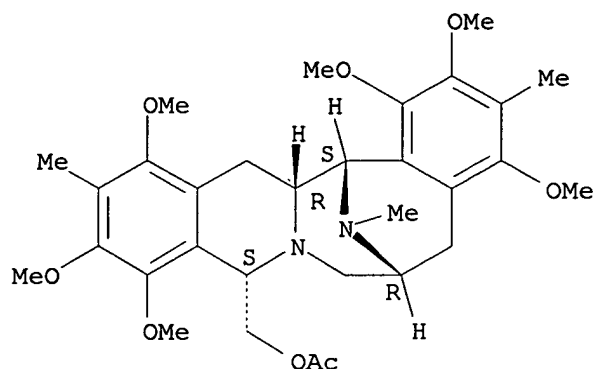
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and demethylation of)

RN 112995-91-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
acetate (ester), (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.

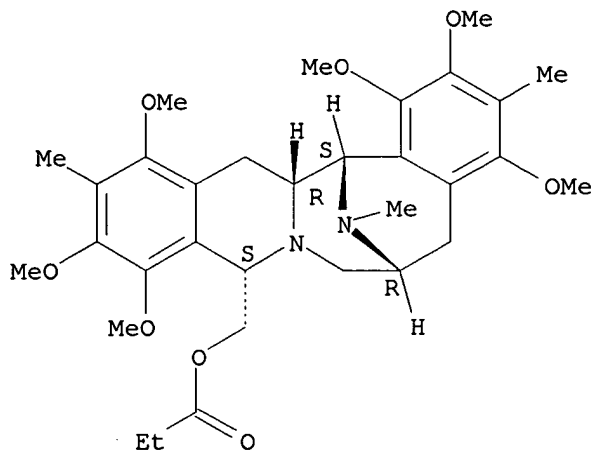
10/826,859



RN 136581-76-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
propanoate (ester), (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.



IT 136604-12-1P

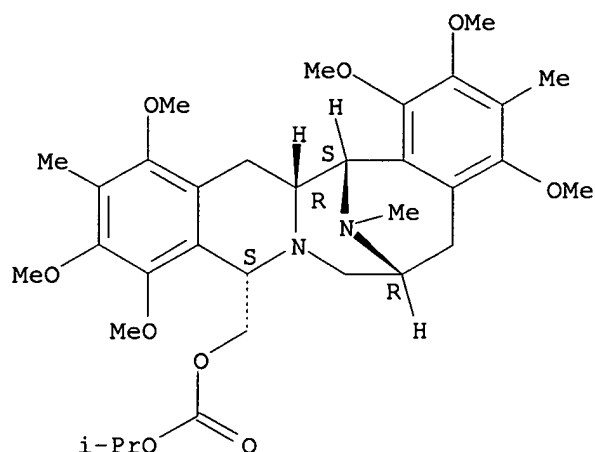
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and hydrolysis of)

RN 136604-12-1 CAPLUS

CN Carbonic acid, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-  
3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl  
1-methylethyl ester, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.

10/826,859



IT 112529-59-6P

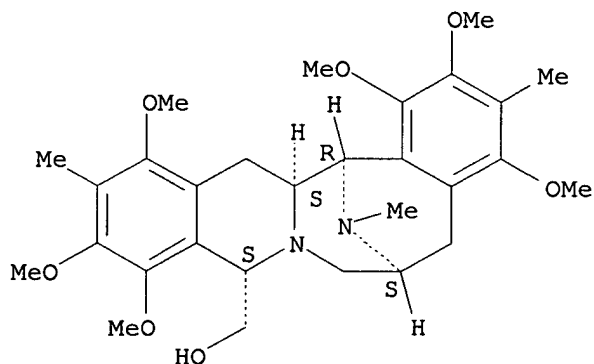
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with phthalimide)

RN 112529-59-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 112995-93-4P 136581-72-1P 136581-74-3P

136581-77-6P 136656-91-2P 136656-92-3P

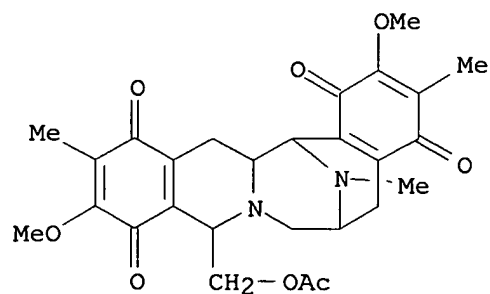
136656-93-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 112995-93-4 CAPLUS

CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(9H)-tetrone,  
9-[(acetyloxy)methyl]-5,6,7,14,14a,15-hexahydro-2,11-dimethoxy-3,12,16-  
trimethyl-, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

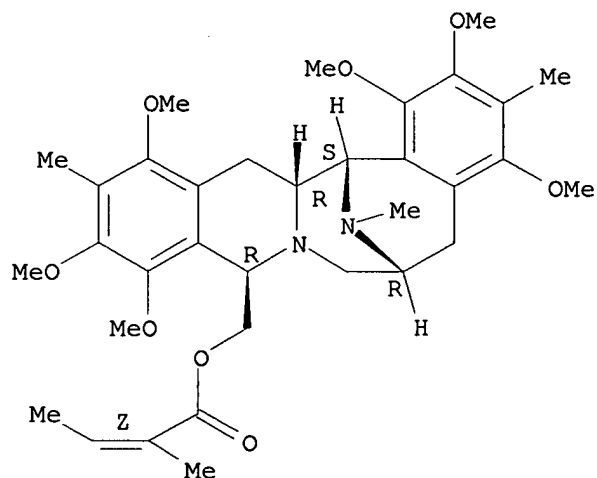
10/826,859



RN 136581-72-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6 $\alpha$ ,9 $\alpha$ (Z),14 $\alpha$ ,15 $\alpha$ ]- (9CI) (CA INDEX NAME)

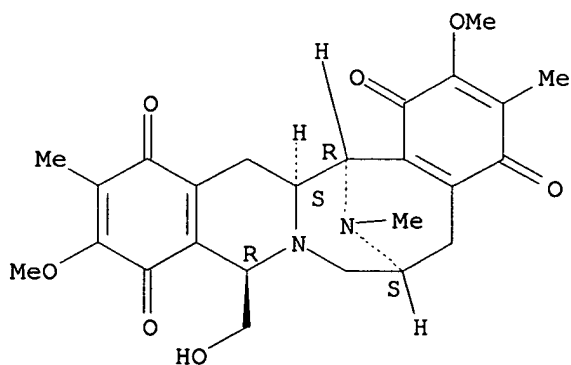
Relative stereochemistry.  
Double bond geometry as shown.



RN 136581-74-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-1,4,10,13-tetrone, 6,7,9,14,14a,15-hexahydro-9-(hydroxymethyl)-2,11-dimethoxy-3,12,16-trimethyl-, (6R,9S,14aR,15S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

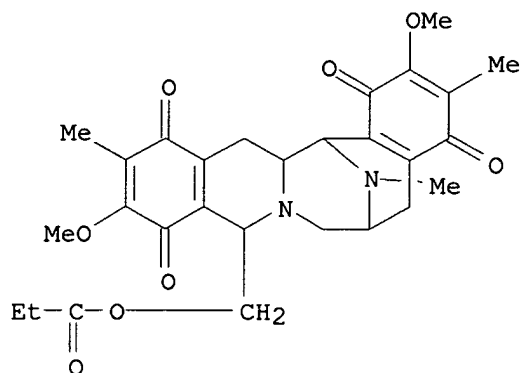




10/826,859

RN 136581-77-6 CAPLUS

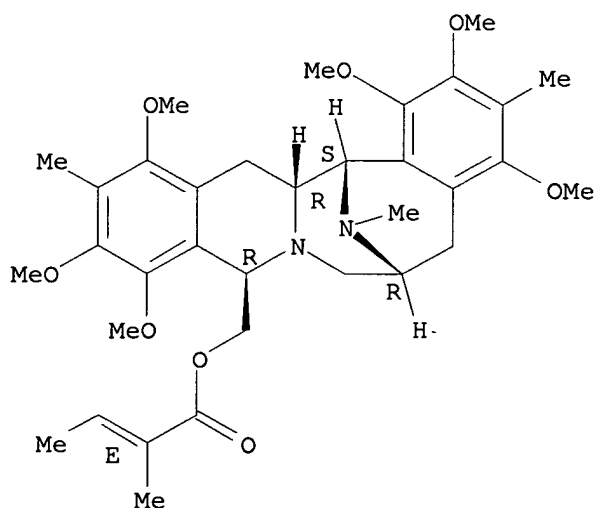
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-1,4,10,13-tetrone,  
6,7,9,14,14a,15-hexahydro-2,11-dimethoxy-3,12,16-trimethyl-9-[(1-oxopropoxy)methyl]-, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA  
INDEX NAME)



RN 136656-91-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6 $\alpha$ ,9 $\alpha$ (E),14 $\alpha\alpha$ ,15 $\alpha$ ]- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.

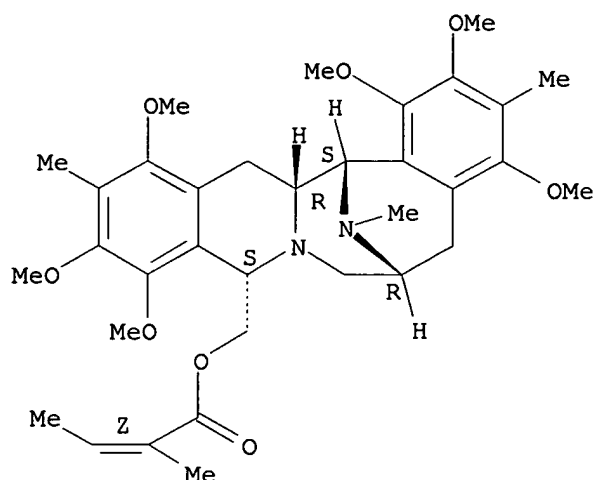


RN 136656-92-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6 $\alpha$ ,9 $\beta$ (Z),14 $\alpha\alpha$ ,15 $\alpha$ ]- (9CI) (CA  
INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.

10/826,859

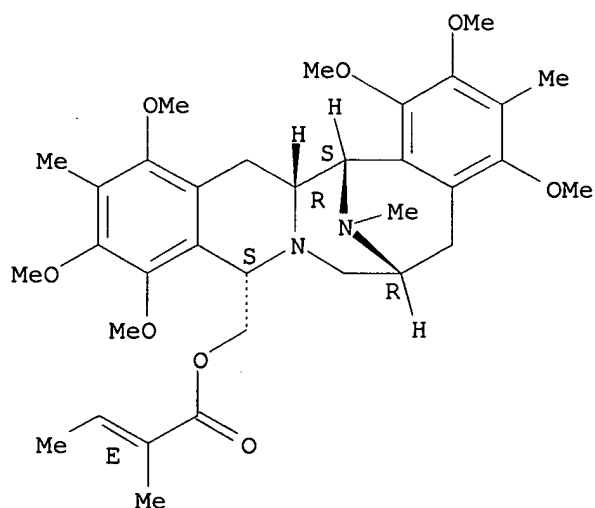


RN 136656-93-4 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [6 $\alpha$ ,9 $\beta$ (E),14 $\alpha\alpha$ ,15 $\alpha$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry as shown.



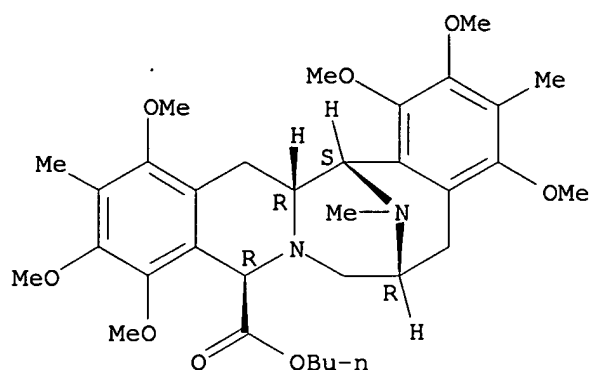
IT 112529-58-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(reduction of)

RN 112529-58-5 CAPLUS

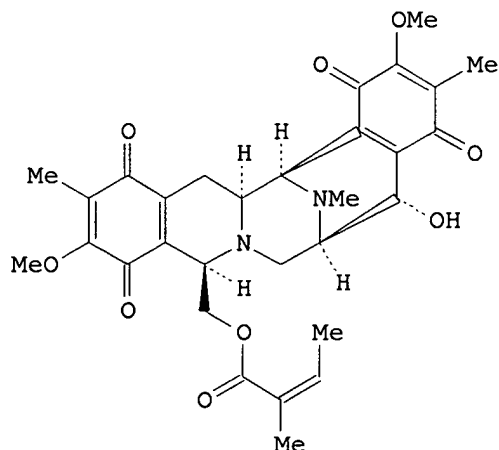
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



1449

L7 ANSWER 20 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1991:102523 CAPLUS  
 DOCUMENT NUMBER: 114:102523  
 TITLE: A stereocontrolled total synthesis of  
 (±)-renieramycin A  
 AUTHOR(S): Fukuyama, Tohru; Linton, Steven D.; Tun, Min Min  
 CORPORATE SOURCE: Dep. Chem., Rice Univ., Houston, TX, 77251, USA  
 SOURCE: Tetrahedron Letters (1990), 31(42), 5989-92  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



I

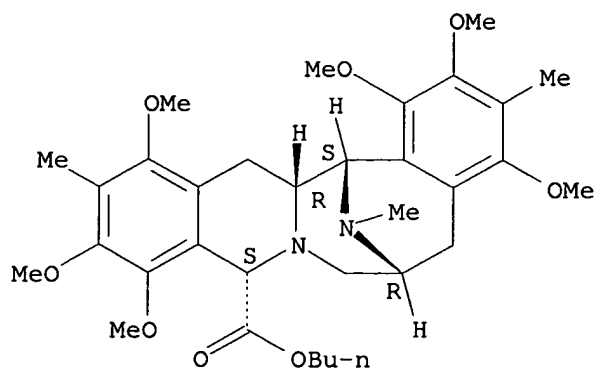
AB The first total synthesis of (±)-renieramycin A (I) is described. The stereochem. of the angelate side chain was unequivocally determined by X-ray crystallog. anal. of the penultimate intermediate.

IT **132340-98-8P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 132340-98-8 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,5,10-trihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5α,6α,9α(2),14a.alpha.a.,15α]- (9CI) (CA INDEX NAME)

10/826,859

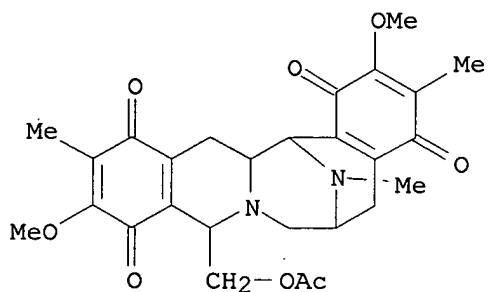


IT 112995-93-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 112995-93-4 CAPLUS

CN 6,15-Imino-4H-isoquino[3,2-b][3]benzazocine-1,4,10,13(9H)-tetrone,  
9-[(acetyloxy)methyl]-5,6,7,14,14a,15-hexahydro-2,11-dimethoxy-3,12,16-  
trimethyl-, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)



L7 ANSWER 25 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:55713 CAPLUS

DOCUMENT NUMBER: 108:55713

TITLE: Studies on the total synthesis of saframycin B

AUTHOR(S): Kobo, Akiyoshi; Saito, Naoki; Yamato, Hidekazu;  
Nakamura, Madoka

CORPORATE SOURCE: Meiji Coll. Pharm., Japan

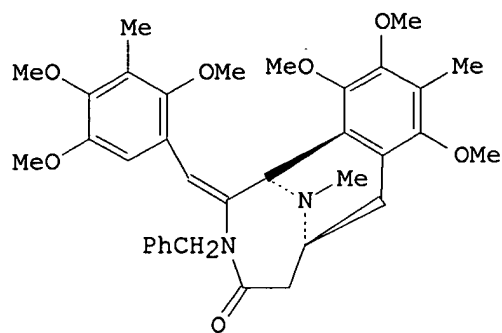
SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1986),  
28th, 465-72

CODEN: TYKYDS

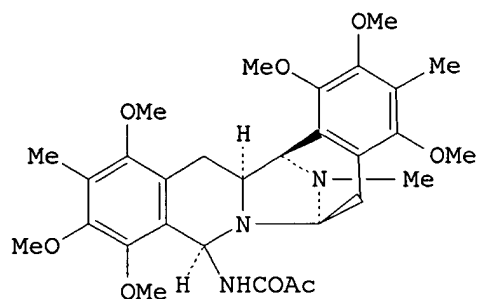
DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



II



III

AB Safamycin B (I) which is an antitumor antibiotic, produced by *Streptomyces lavendulae* were prepared. The preparation of safamycin B intermediate II was reviewed. II was converted into the pentacyclic compound III in 10 steps. Oxidation of III with 10N HNO<sub>3</sub> afforded I in 1% yield. The yield of I was raised to 41% by treatment with BBr<sub>3</sub> at -78° followed by 10N HNO<sub>3</sub>.

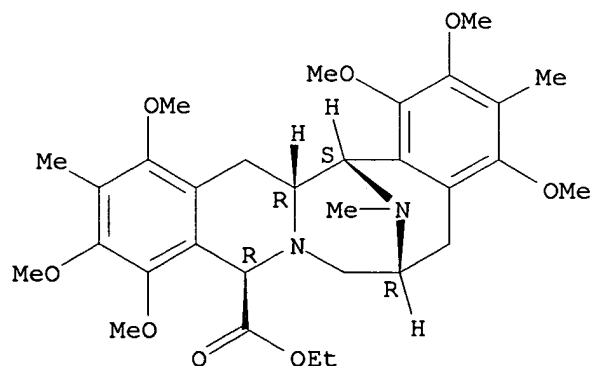
IT **112446-10-3P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
ethyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.



IT **112529-59-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

10/826,859

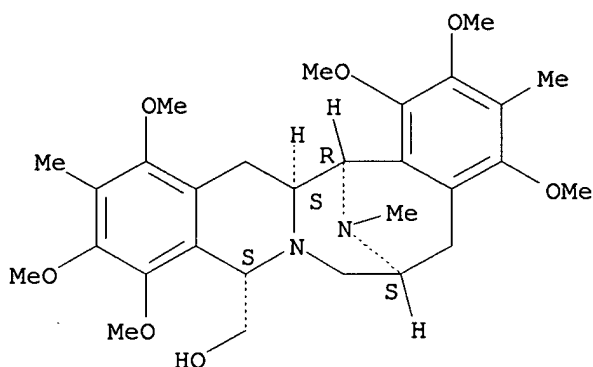
(Reactant or reagent)

(preparation and methylation of)

RN 112529-59-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 112446-11-4P

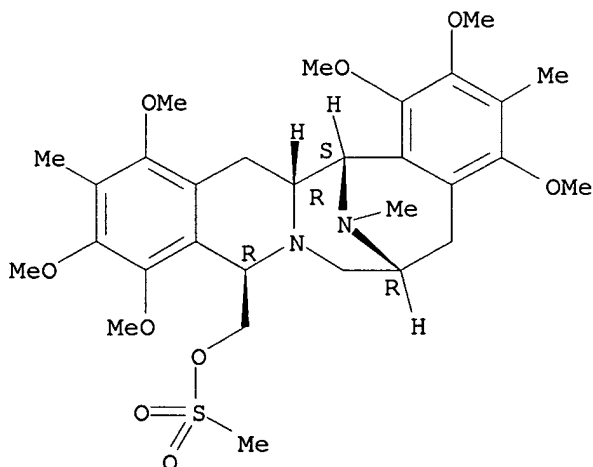
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and reaction of, with azide)

RN 112446-11-4 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
methanesulfonate (ester), (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI)  
(CA INDEX NAME)

Relative stereochemistry.



IT 112446-05-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation and reduction of)

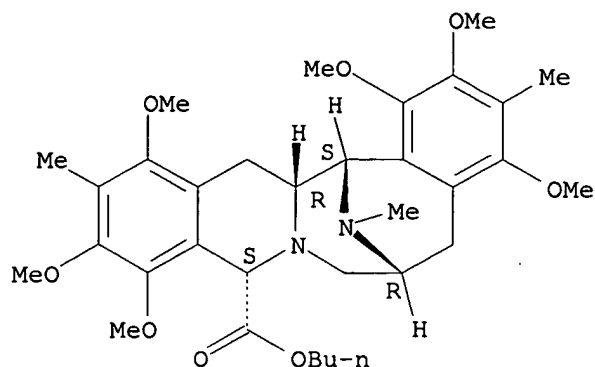
RN 112446-05-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,

10/826,859

6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
butyl ester, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.



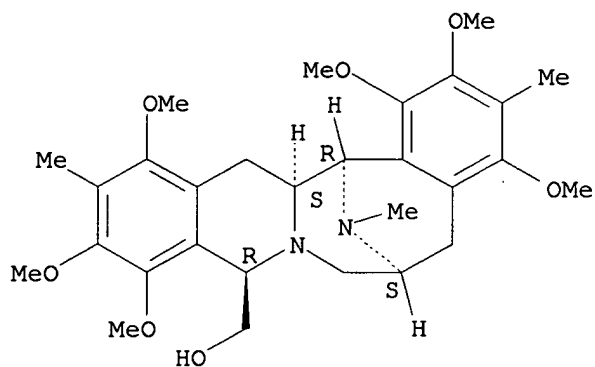
IT 112446-04-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, reaction with phthalimide, hydrazinolysis, and acylation of)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 112529-58-5P

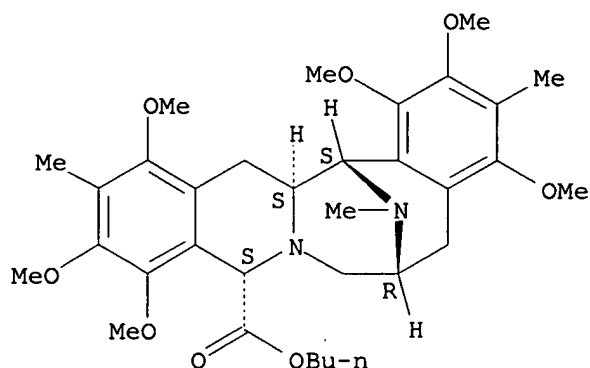
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation, reduction, and isomerization of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
butyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.

10/826,859



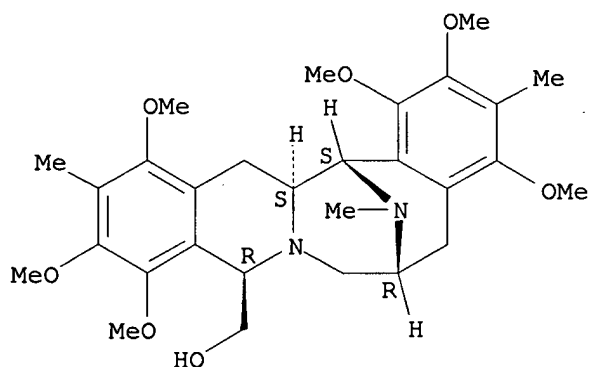
IT 115510-13-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as intermediate for saframycin B)

RN 115510-13-9 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
[6R-(6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$  $\beta$ ,15 $\alpha$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 24 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:112030 CAPLUS

DOCUMENT NUMBER: 108:112030

TITLE: Synthesis of saframycins. I. Total synthesis of  
( $\pm$ )-saframycin B and its congeners

AUTHOR(S): Kubo, Akinori; Saito, Naoki; Yamauchi, Reiko; Sakai,  
Shinichiro

CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1987), 35(5),  
2158-61

CODEN: CPBTAL; ISSN: 0009-2363

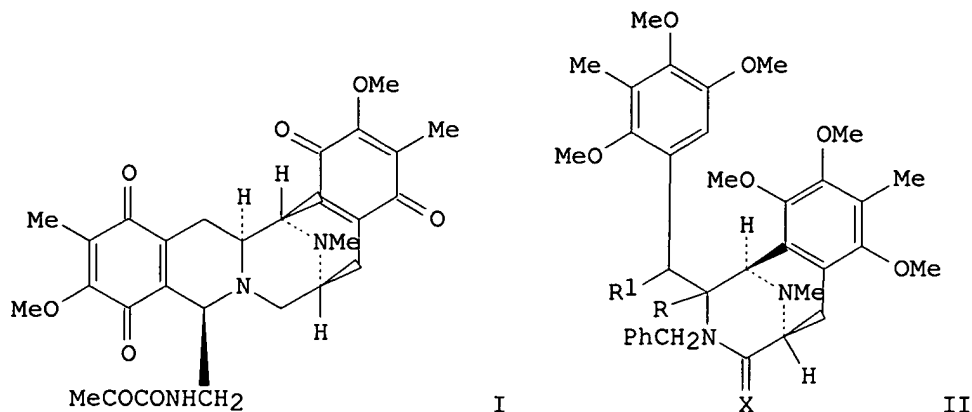
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 108:112030

GI





AB The total synthesis of saframycin B (I) was achieved from tricyclic lactam II (RR1 = bond; X = O). The key step is the stereoselective intramolecular cyclization of the amino acetal II (R = R1 = H; X = H2). The structure of a pentacyclic intermediate was confirmed by x-ray crystallog.

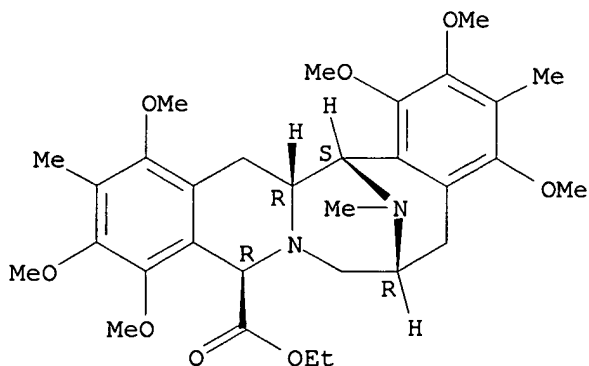
IT **112446-10-3P**

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)

RN 112446-10-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
ethyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.



IT **112995-91-2P**

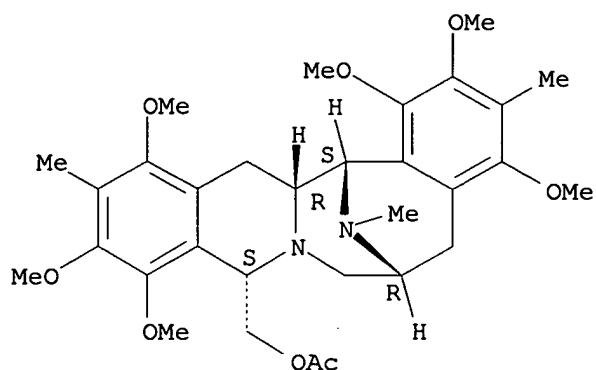
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and demethylation of)

RN 112995-91-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
acetate (ester), (6 $\alpha$ ,9 $\beta$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.

10/826,859



IT **112529-58-5P**

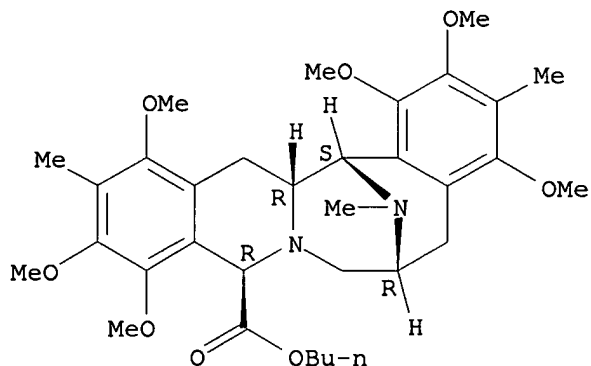
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and epimerization of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT **112446-04-5P 112529-59-6P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

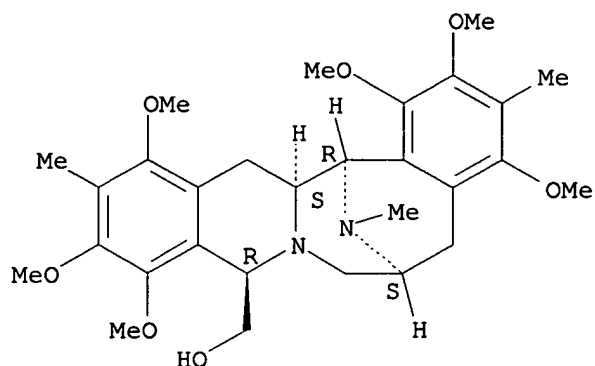
(preparation and reaction of, with phthalimide)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.

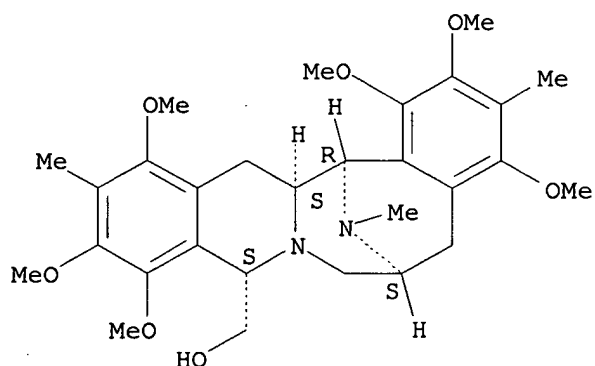
10/826,859



RN 112529-59-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 112446-05-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation and reduction of)

RN 112446-05-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
butyl ester, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.

the first naturally occurring isoindole to be described, was confirmed by an unambiguous synthesis. The structures of the renieramycins were determined by anal. of spectral data, especially  $^1\text{H}$  NMR. All the compds. showed antimicrobial activity.

IT 79664-60-1 79664-61-2 79664-62-3

79664-63-4

RL: BOC (Biological occurrence); BSU (Biological study, unclassified);

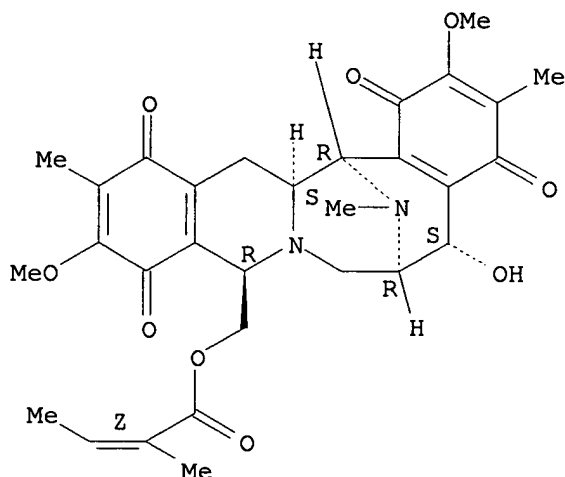
BIOL (Biological study); OCCU (Occurrence)

(of sponge)

RN 79664-60-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

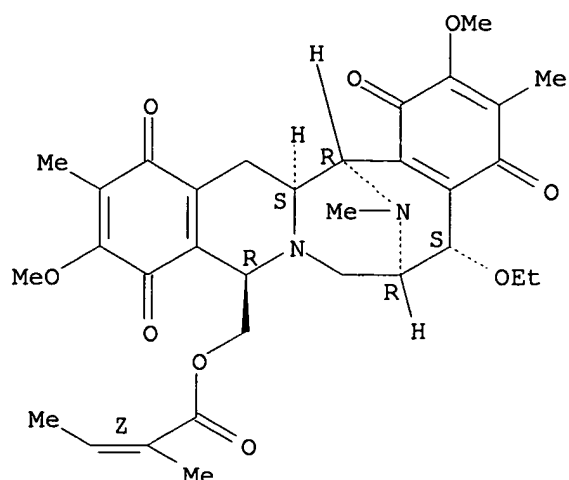


RN 79664-61-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-5-ethoxy-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

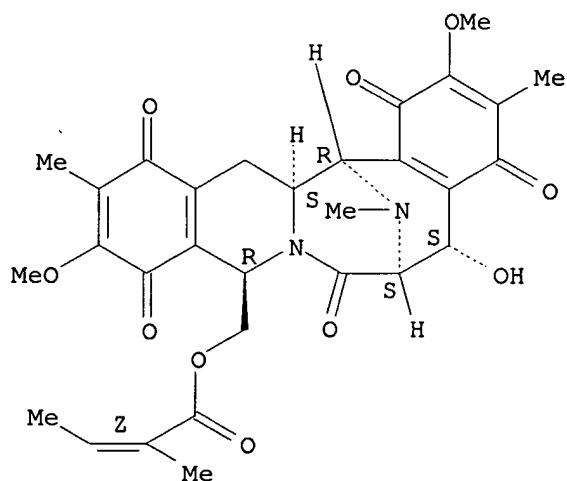
10/826,859



RN 79664-62-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

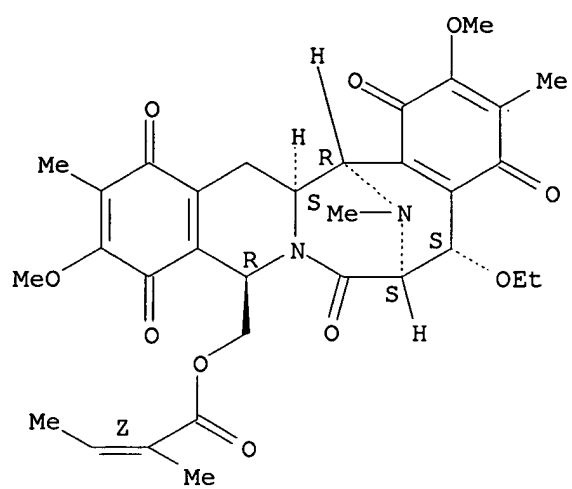


RN 79664-63-4 CAPLUS

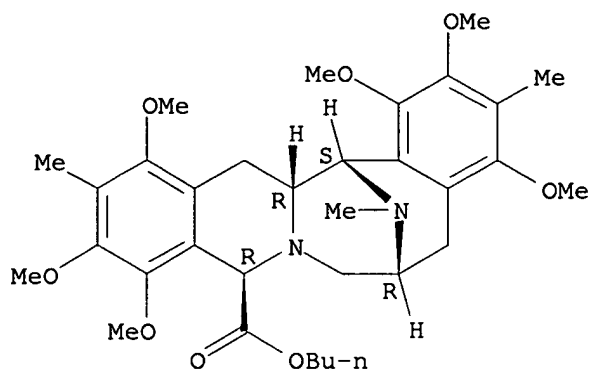
CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-5-ethoxy-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

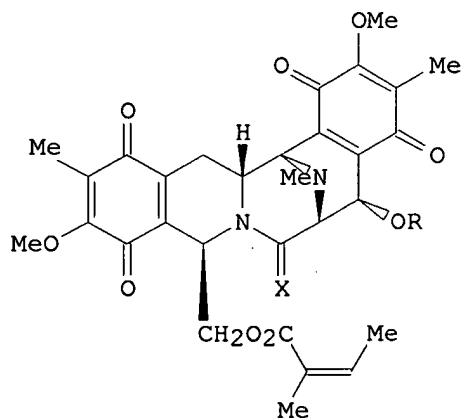
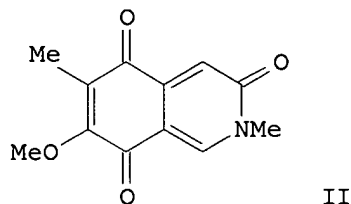
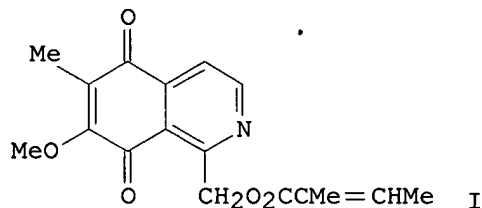
10/826,859



=>



L7 ANSWER 26 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1982:31904 CAPLUS  
 DOCUMENT NUMBER: 96:31904  
 TITLE: Antimicrobial metabolites of the sponge *Reniera* sp  
 AUTHOR(S): Frincke, James M.; Faulkner, D. John  
 CORPORATE SOURCE: Scripps Inst. Oceanogr., La Jolla, CA, 92093, USA  
 SOURCE: Journal of the American Chemical Society (1982),  
 104(1), 265-9  
 CODEN: JACSAT; ISSN: 0002-7863  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

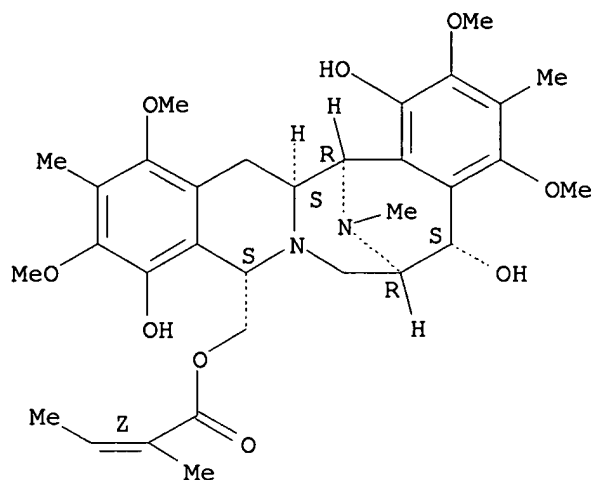


IV, R=H, X=2H  
 V, R=Et, X=2H  
 VI, R=H, X=O  
 VII, R=Et, X=O

AB The sponge *Reniera* contains renierone (I), mimosamycin (II),  
 N-formyl-1,2-dihydrorenierone, O-demethylrenierone, 1,6-dimethyl-7-methoxy-  
 5,8-dihydroisoquinoline-5,8-dione, 2,5-dimethyl-6-methoxy-4,7-  
 dihydroisoindole-4,7-dione (III), and renieramycins A-D (IV-VII). III,

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Relative stereochemistry.  
Double bond geometry as shown.



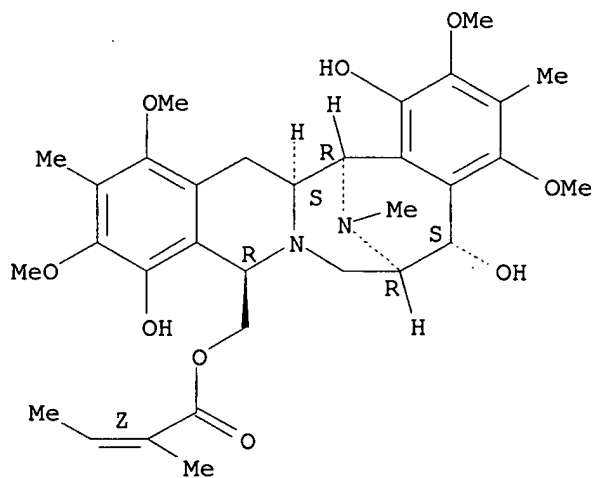
IT 132277-62-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, crystal structure, and oxidation of)

RN 132277-62-4 CAPLUS

CN 2-Butenoic acid, 2-methyl-, (6,7,9,14,14a,15-hexahydro-1,5,10-trihydroxy-2,4,11,13-tetramethoxy-3,12,16-trimethyl-6,15-imino-5H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5 $\alpha$ ,6 $\alpha$ ,9 $\beta$ (Z),14a.alpha.,15 $\alpha$ ]- (9CI) (CA INDEX NAME)

Relative stereochemistry.  
Double bond geometry as shown.



IT 132342-06-4P, ( $\pm$ )-Renieramycin A

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(stereocontrolled total synthesis of)

RN 132342-06-4 CAPLUS

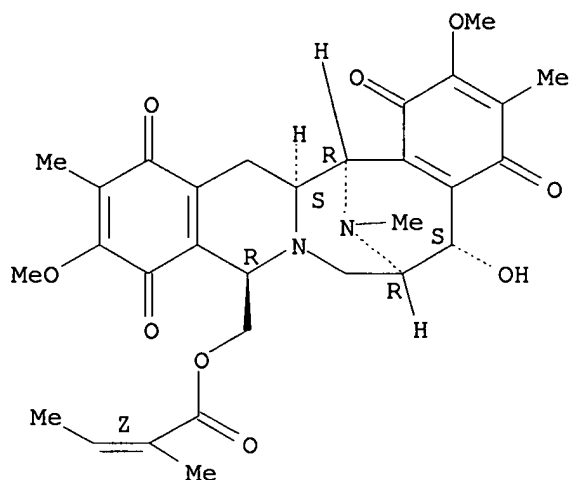
CN 2-Butenoic acid, 2-methyl-, (1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, [5 $\alpha$ ,6 $\alpha$ ,9 $\beta$ (Z),14a.alpha.,15 $\alpha$ ]- (9CI) (CA INDEX NAME)



10/826,859

isoquino[3,2-b][3]benzazocin-9-yl)methyl ester,  
[5 $\alpha$ ,6 $\alpha$ ,9 $\beta$ (Z),14 $\alpha\alpha$ ,15 $\alpha$ ]- (9CI) (CA INDEX  
NAME)

Relative stereochemistry.  
Double bond geometry as shown.



L7 ANSWER 21 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:4919 CAPLUS

DOCUMENT NUMBER: 112:4919

TITLE: Renieramycins E and F from the sponge Reniera sp.:  
reassignment of the stereochemistry of the  
renieramycins

AUTHOR(S): He, Hai Yin; Faulkner, D. John

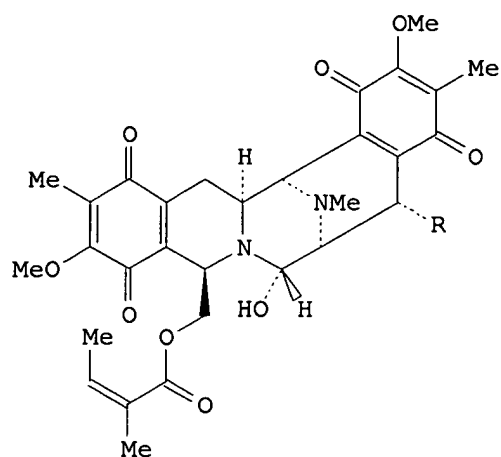
CORPORATE SOURCE: Scripps Inst. Oceanogr., Univ. California, La Jolla,  
CA, 92093, USA

SOURCE: Journal of Organic Chemistry (1989), 54(24), 5822-4  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

AB Renieramycins E (I, R = H) and F (I, R = MeO) are two very unstable alkaloids from the sponge *Reniera* sp. collected in Palau. The structure and stereochem. of renieramycins E and F were established by interpretation of spectral data. The stereochem. of renieramycin E is the same as that of the saframycins and there is good evidence to support reassignment of the stereochem. of all renieramycins. The facile decomposition of renieramycins E and F is discussed.

IT 79664-60-1 79664-61-2 79664-62-3

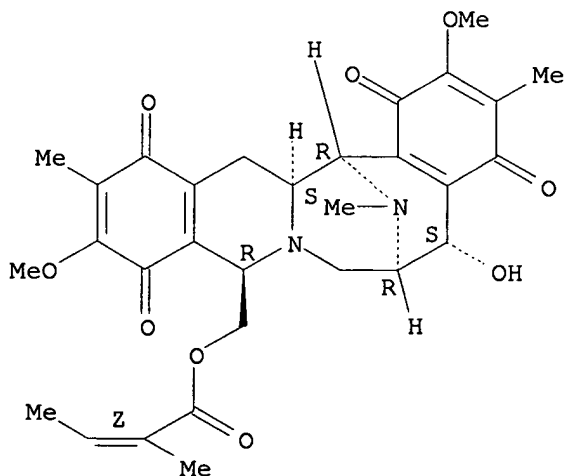
79664-63-4

RL: PRP (Properties)  
(configuration of)

RN 79664-60-1 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



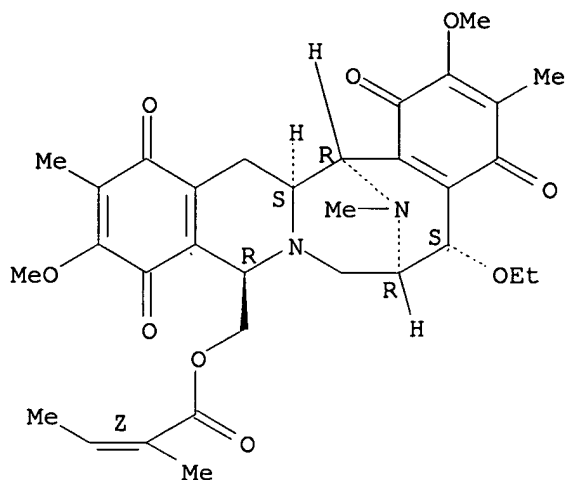
RN 79664-61-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6R,9R,14aS,15R)-5-ethoxy-

10/826,859

1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-  
1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl  
ester, (2Z)- (9CI) (CA INDEX NAME)

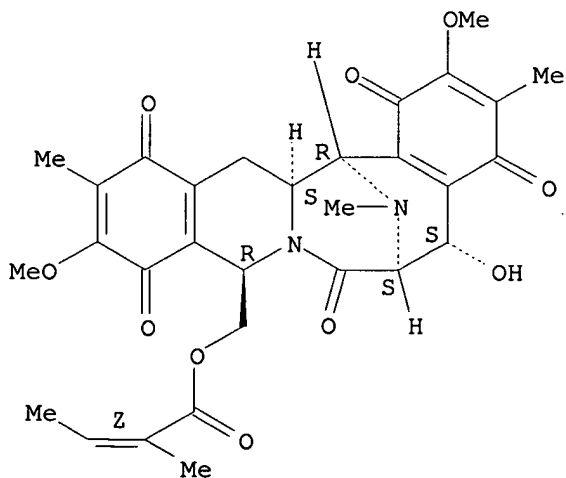
Absolute stereochemistry.  
Double bond geometry as shown.



RN 79664-62-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-5-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.

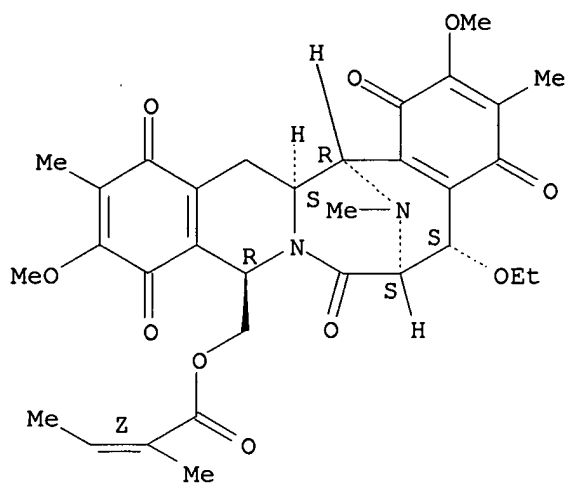


RN 79664-63-4 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,9R,14aS,15R)-5-ethoxy-1,5,6,7,9,10,13,14,14a,15-decahydro-2,11-dimethoxy-3,12,16-trimethyl-1,4,7,10,13-pentaoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl)methyl ester, (2Z)- (9CI) (CA INDEX NAME)

10/826,859

Absolute stereochemistry.  
Double bond geometry as shown.



IT 123641-95-2 123641-96-3

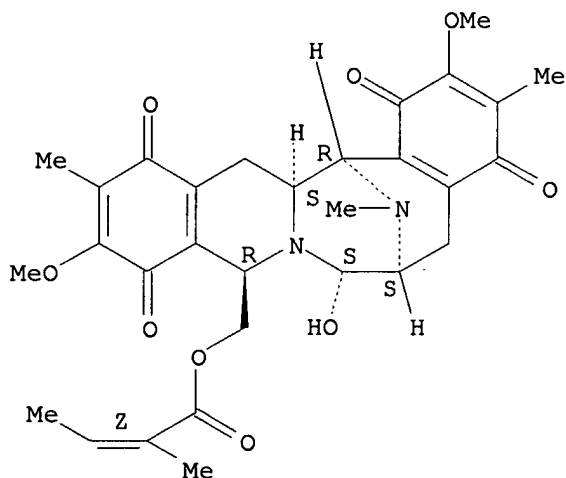
RL: BIOL (Biological study)

(isolation, mol. structure, and configuration of)

RN 123641-95-2 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,11-dimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.  
Double bond geometry as shown.



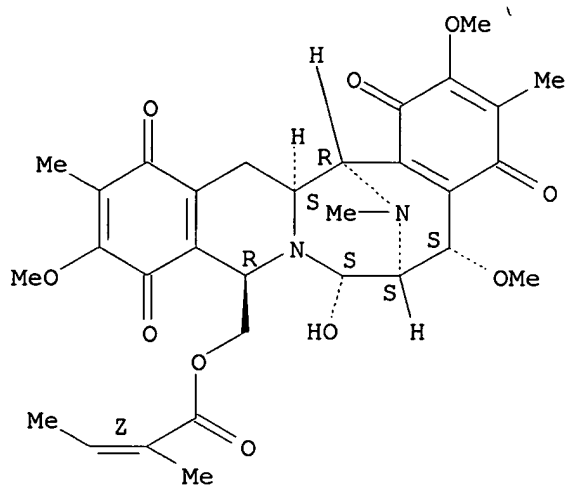
RN 123641-96-3 CAPLUS

CN 2-Butenoic acid, 2-methyl-, [(5S,6S,7S,9R,14aS,15R)-1,5,6,7,9,10,13,14,14a,15-decahydro-7-hydroxy-2,5,11-trimethoxy-3,12,16-trimethyl-1,4,10,13-tetraoxo-6,15-imino-4H-isoquino[3,2-b][3]benzazocin-9-yl]methyl ester, (2Z)- (9CI) (CA INDEX NAME)

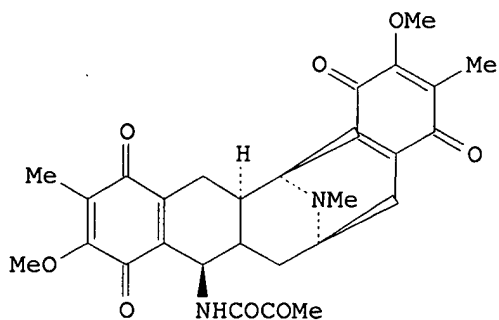
Absolute stereochemistry.

10/826,859

Double bond geometry as shown.



L7 ANSWER 22 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1988:510118 CAPLUS  
DOCUMENT NUMBER: 109:110118  
TITLE: Stereoselective total synthesis of (±)-saframycin B  
AUTHOR(S): Kubo, Akinori; Saito, Naoki; Yamato, Hidekazu;  
Masubuchi, Kazunao; Nakamura, Madoka  
CORPORATE SOURCE: Meiji Coll. Pharm., Tokyo, 154, Japan  
SOURCE: Journal of Organic Chemistry (1988), 53(18), 4295-310  
CODEN: JOCEAH; ISSN: 0022-3263  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 109:110118  
GI

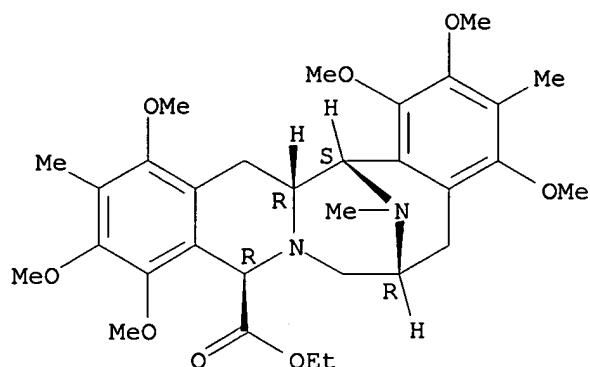


AB A 20-step total synthesis of (±)-saframycin B (I) from  
(Z)-1-acetyl-3-arylidene-6-(arylmethyl)-2,5-piperazinedione is described.  
IT 112446-10-3P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and crystal structure of)  
RN 112446-10-3 CAPLUS  
CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
ethyl ester, (6α,9α,14α,15α)- (9CI) (CA INDEX

10/826,859

NAME)

Relative stereochemistry.



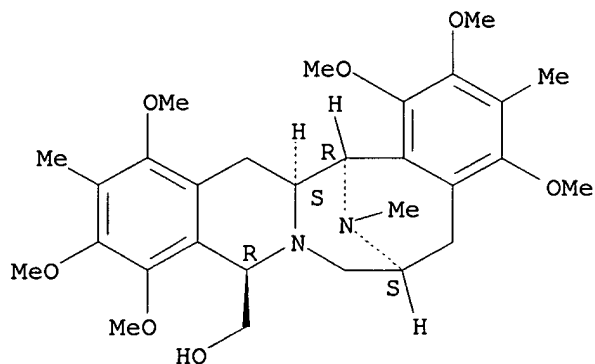
IT 112446-04-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reaction of, with phthalimide)

RN 112446-04-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-methanol,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
(6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )-(9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 112446-05-6P

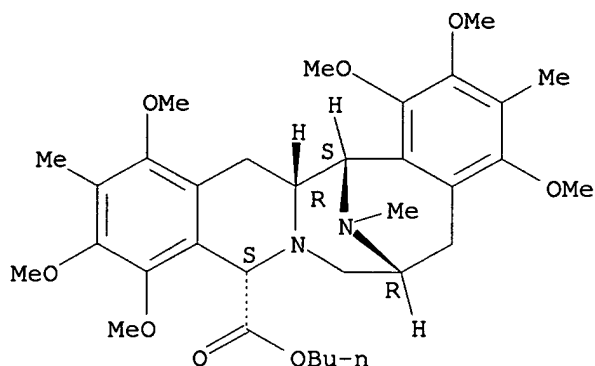
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reduction of)

RN 112446-05-6 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid,  
6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-,  
butyl ester, (6 $\alpha$ ,9 $\beta$ ,14 $\alpha\alpha$ ,15 $\alpha$ )-(9CI) (CA INDEX NAME)

Relative stereochemistry.

10/826,859



IT 112529-58-5P

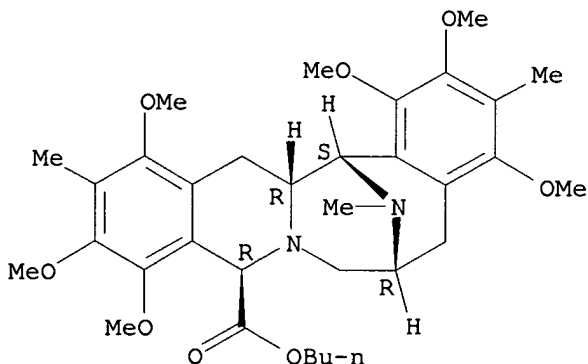
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and transesterification of)

RN 112529-58-5 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, (6 $\alpha$ ,9 $\alpha$ ,14 $\alpha$ ,15 $\alpha$ )- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L7 ANSWER 23 OF 26 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:473253 CAPLUS

DOCUMENT NUMBER: 109:73253

TITLE: Preparation of 6,15-iminoisoquino[3,2-b][3]benzazocine derivatives as intermediates for an antitumor agent saframycin B

INVENTOR(S): Kubo, Yotoku; Saito, Naoki

PATENT ASSIGNEE(S): Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

JP 63002991	A2	19880107	JP 1986-144916	19860623
PRIORITY APPLN. INFO.:			JP 1986-144916	19860623
OTHER SOURCE(S):	MARPAT 109:73253			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Isoquinolines I (R = CH<sub>2</sub>OH, CH<sub>2</sub>NH<sub>2</sub>, phthaloylmethyl) (II) are prepared from diazabicyclononane III. A mixture of III and K<sub>2</sub>CO<sub>3</sub> in BuOH was treated with OHCCO<sub>2</sub>Bu at room temperature for 67 h and the concentrated reaction mixture was stirred

in CF<sub>3</sub>CO<sub>2</sub>H at ice-cooled temperature for 1 h to give 70.2% isoquinoline IV, which was isomerized by treatment with Hg(OAc)<sub>2</sub> in AcOH and then H<sub>2</sub>S(g), followed by NaBH<sub>4</sub> treatment of the product in EtOH in the presence of NaHCO<sub>3</sub> to give 70.6% I (R = CO<sub>2</sub>Bu) (V). A mixture of V and LiAlH<sub>4</sub> in THF was refluxed for 2 h to afford 76.8% I (R = CH<sub>2</sub>OH), which was converted to saframycin B in 4 steps.

IT 115510-17-3P

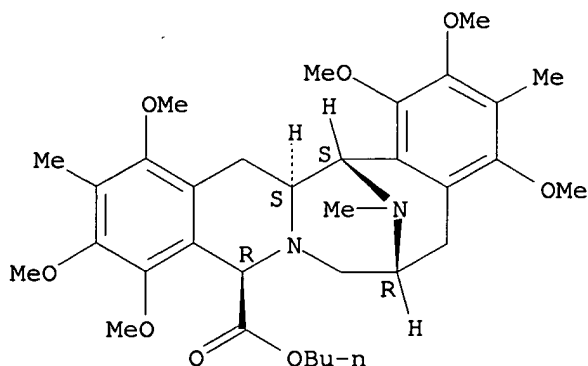
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and LAH reduction of, in preparation of saframycin B)

RN 115510-17-3 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, [6R-(6 $\alpha$ ,9 $\alpha$ ,14a $\beta$ ,15 $\alpha$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 115510-16-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and isomerization of, in preparation of saframycin B)

RN 115510-16-2 CAPLUS

CN 6,15-Imino-5H-isoquino[3,2-b][3]benzazocine-9-carboxylic acid, 6,7,9,14,14a,15-hexahydro-1,2,4,10,11,13-hexamethoxy-3,12,16-trimethyl-, butyl ester, [6R-(6 $\alpha$ ,9 $\beta$ ,14a $\beta$ ,15 $\alpha$ )]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.